Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 07:31 am GMT

PDB ID	:	2BFA
Title	:	Leishmania major pteridine reductase 1 in complex with NADP and CB3717
Authors	:	Schuettelkopf, A.W.; Hunter, W.N.
Deposited on	:	2004-12-06
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

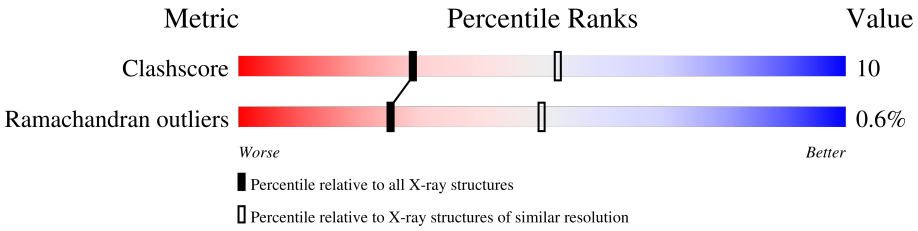
MolProbity	:	4.02b-467
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	288	75% 17% 8%
1	B	288	73% 18% • 8%
1	C	288	73% 14% 12%
1	D	288	73% 15% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	1291	-	-	X	-
4	EDO	A	1293	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	1291	-	-	X	-
4	EDO	D	1291	-	-	X	-
4	EDO	D	1292	-	-	X	-

2 Entry composition (i)

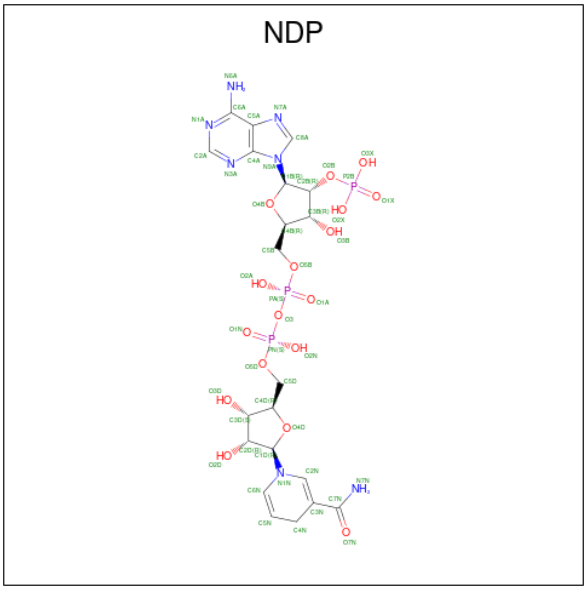
There are 5 unique types of molecules in this entry. The entry contains 8319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1980	1248	352	369	11			
1	B	266	Total	C	N	O	S	0	0	0
			1984	1250	353	370	11			
1	C	253	Total	C	N	O	S	0	0	0
			1885	1189	337	349	10			
1	D	255	Total	C	N	O	S	0	0	0
			1903	1199	341	353	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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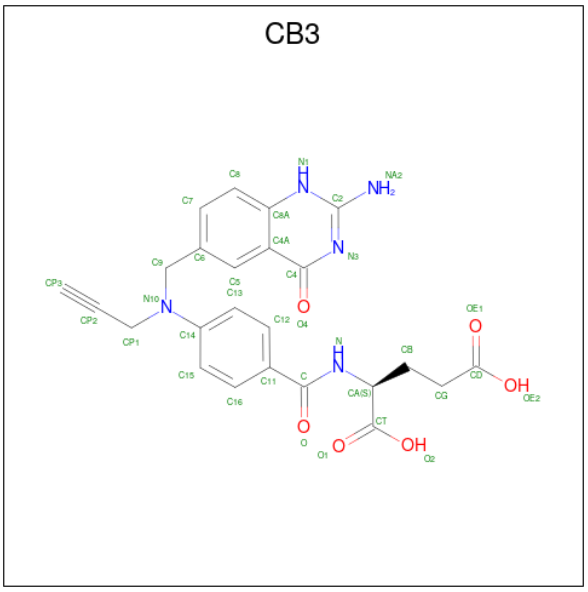
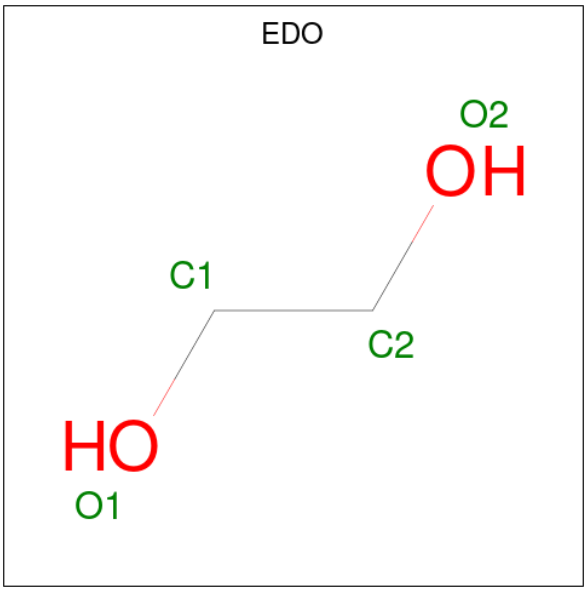
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	42	Total O 42 42	0	0
5	C	63	Total O 63 63	0	0
5	D	47	Total O 47 47	0	0

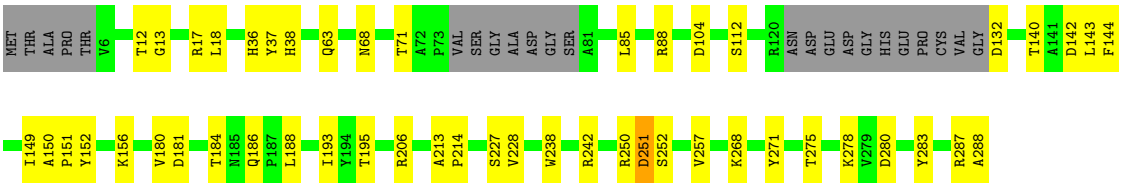
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS failed to run properly.

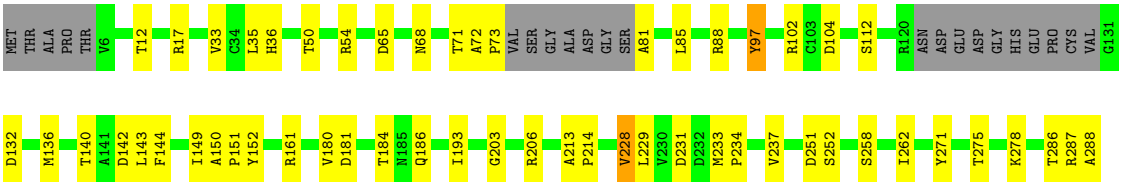
• Molecule 1: PTERIDINE REDUCTASE 1

Chain A:



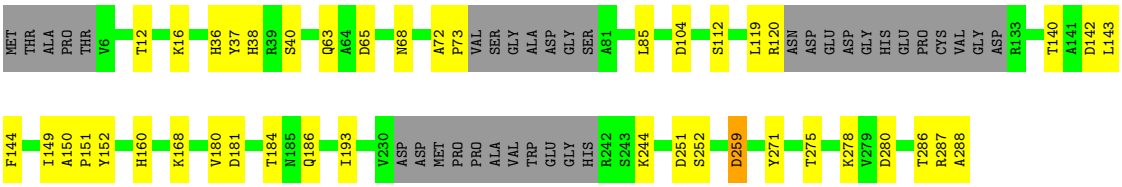
• Molecule 1: PTERIDINE REDUCTASE 1

Chain B:



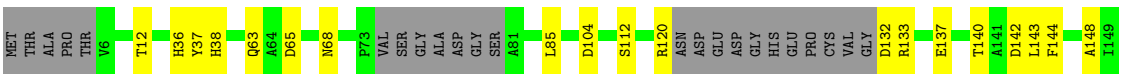
• Molecule 1: PTERIDINE REDUCTASE 1

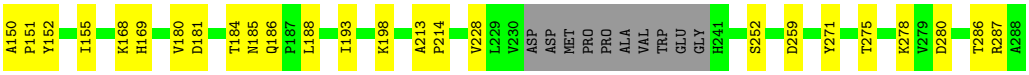
Chain C:



• Molecule 1: PTERIDINE REDUCTASE 1

Chain D:




A150
P151
Y152
I155
K168
H169
V180
D181
T184
N185
Q186
P187
L188
I193
K198
A213
P214
V228
L229
V230
ASP
ASP
MET
PRO
PRO
ALA
VAL
TRP
GLU
GLY
H241
S252
D259
Y271
T275
K278
V279
D280
T286
R287
A288

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.54Å 103.83Å 137.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.50 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (24.50-2.70)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.236	Depositor
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.191	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8319	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 29.00 % 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 1.6721e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, NDP, CB3

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	0.40	0/2019	0.65	5/2750 (0.2%)
1	B	0.46	2/2023 (0.1%)	0.64	6/2755 (0.2%)
1	C	0.40	0/1918	0.62	6/2608 (0.2%)
1	D	0.43	0/1937	0.63	5/2634 (0.2%)
All	All	0.42	2/7897 (0.0%)	0.64	22/10747 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	TYR	CE1-CZ	-5.88	1.30	1.38
1	B	97	TYR	CE2-CZ	-5.64	1.31	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	104	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	104	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	104	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	104	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	132	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	231	ASP	CB-CG-OD2	5.53	123.27	118.30
1	D	280	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	65	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	132	ASP	CB-CG-OD2	5.35	123.12	118.30
1	C	251	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	142	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	251	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	142	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	142	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	65	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	259	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	280	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	280	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	142	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	259	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	251	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1980	0	1987	46	0
1	B	1984	0	1990	55	0
1	C	1885	0	1911	36	0
1	D	1903	0	1922	36	0
2	A	48	0	26	1	0
2	B	48	0	26	2	0
2	C	48	0	26	1	0
2	D	48	0	26	2	0
3	A	35	0	21	7	0
3	B	35	0	21	6	0
3	C	35	0	21	4	0
3	D	35	0	21	7	0
4	A	12	0	18	16	0
4	B	4	0	6	7	0
4	D	8	0	12	12	0
5	A	59	0	0	1	0
5	B	42	0	0	1	0
5	C	63	0	0	1	0
5	D	47	0	0	1	0
All	All	8319	0	8034	156	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 10.

All (156) 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:B:68:ASN:HD22	4:B:1291:EDO:H21	1.17	1.07
1:B:275:THR:HG21	1:D:278:LYS:HB2	1.43	0.99
1:A:278:LYS:HB2	1:C:275:THR:HG21	1.46	0.98
3:A:1290:CB3:H12	1:D:287:ARG:HH21	1.27	0.97
1:C:149:ILE:CD1	4:D:1292:EDO:H21	1.95	0.96
1:D:188:LEU:HD22	4:D:1291:EDO:H21	1.46	0.96
1:B:278:LYS:HB2	1:D:275:THR:HG21	1.49	0.93
1:A:188:LEU:HD22	4:A:1291:EDO:H21	1.53	0.90
1:A:275:THR:HG21	1:C:278:LYS:HB2	1.51	0.89
1:B:68:ASN:ND2	4:B:1291:EDO:H21	1.89	0.86
1:B:12:THR:HA	1:B:36:HIS:HB3	1.56	0.85
3:A:1290:CB3:H12	1:D:287:ARG:NH2	1.93	0.84
1:D:68:ASN:HD22	4:D:1292:EDO:H12	1.42	0.84
1:A:287:ARG:HH21	3:D:1290:CB3:H12	1.43	0.83
3:A:1290:CB3:H13	4:A:1291:EDO:O2	1.77	0.83
1:A:181:ASP:OD2	4:A:1291:EDO:H12	1.79	0.82
1:C:149:ILE:HD11	4:D:1292:EDO:H21	1.65	0.79
1:A:287:ARG:NH2	3:D:1290:CB3:H12	1.97	0.78
1:B:68:ASN:HD22	4:B:1291:EDO:C2	1.96	0.77
4:A:1293:EDO:H21	1:B:203:GLY:CA	2.14	0.77
1:B:287:ARG:HH21	3:C:1290:CB3:H12	1.50	0.76
1:A:186:GLN:O	1:D:287:ARG:NH1	2.21	0.73
1:A:195:THR:CG2	4:A:1293:EDO:H12	2.17	0.73
1:A:242:ARG:NH1	1:A:251:ASP:OD1	2.23	0.72
1:B:17:ARG:NH1	1:B:228:VAL:HG23	2.05	0.72
1:C:168:LYS:HD3	1:C:168:LYS:H	1.53	0.71
1:B:97:TYR:CE1	1:B:102:ARG:HA	2.26	0.71
1:C:12:THR:HA	1:C:36:HIS:HB3	1.74	0.69
1:C:181:ASP:HB3	1:C:184:THR:HG23	1.73	0.69
1:A:287:ARG:NH1	1:D:186:GLN:O	2.26	0.68
4:A:1293:EDO:H21	1:B:203:GLY:HA3	1.74	0.67
1:D:12:THR:HA	1:D:36:HIS:HB3	1.77	0.67
1:C:112:SER:HB2	1:C:143:LEU:HD23	1.77	0.67
1:B:228:VAL:HG23	1:B:228:VAL:O	1.94	0.67
1:A:112:SER:HB2	1:A:143:LEU:HD23	1.74	0.67
1:D:181:ASP:HB3	1:D:184:THR:HG23	1.75	0.66
1:B:112:SER:HB2	1:B:143:LEU:HD23	1.77	0.66
1:A:12:THR:HA	1:A:36:HIS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1290:CB3:H13	5:C:2057:HOH:O	1.94	0.66
3:B:1290:CB3:H12	1:C:287:ARG:NH2	2.10	0.66
1:D:112:SER:HB2	1:D:143:LEU:HD23	1.79	0.65
1:D:133:ARG:O	1:D:137:GLU:HG2	1.97	0.65
1:A:252:SER:HB3	1:C:271:TYR:CE2	2.32	0.65
3:B:1290:CB3:H12	1:C:287:ARG:HH21	1.63	0.64
1:D:68:ASN:ND2	4:D:1292:EDO:H12	2.12	0.64
1:A:242:ARG:HB3	1:A:250:ARG:HA	1.81	0.63
3:A:1290:CB3:H7	4:A:1291:EDO:H22	1.79	0.63
1:A:288:ALA:HB2	1:D:286:THR:HB	1.82	0.62
1:B:229:LEU:HD11	3:B:1290:CB3:H15	1.81	0.62
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.82	0.62
1:A:181:ASP:HB3	1:A:184:THR:HG23	1.81	0.61
1:B:97:TYR:CE2	1:B:161:ARG:HB3	2.35	0.61
1:B:287:ARG:NH2	3:C:1290:CB3:H12	2.15	0.61
3:D:1290:CB3:H7	4:D:1291:EDO:H22	1.82	0.61
1:B:287:ARG:NH1	1:C:186:GLN:O	2.31	0.60
1:D:150:ALA:HB3	1:D:151:PRO:HD3	1.83	0.60
3:A:1290:CB3:C7	4:A:1291:EDO:H22	2.31	0.60
1:A:150:ALA:HB3	1:A:151:PRO:HD3	1.84	0.60
1:B:288:ALA:HB2	1:C:286:THR:HB	1.83	0.59
1:B:186:GLN:O	1:C:287:ARG:NH1	2.33	0.59
1:A:149:ILE:HD11	4:B:1291:EDO:H12	1.85	0.59
1:A:271:TYR:CE2	1:C:252:SER:HB3	2.38	0.58
4:A:1293:EDO:H21	1:B:203:GLY:HA2	1.85	0.58
1:A:278:LYS:HB2	1:C:275:THR:CG2	2.29	0.58
1:B:271:TYR:CE2	1:D:252:SER:HB3	2.38	0.58
1:A:195:THR:HG22	4:A:1293:EDO:H12	1.85	0.57
1:B:150:ALA:HB3	1:B:151:PRO:HD3	1.84	0.57
1:C:193:ILE:HD11	1:D:152:TYR:CE2	2.40	0.57
1:D:132:ASP:OD1	1:D:132:ASP:C	2.43	0.57
1:A:206:ARG:HH22	4:A:1292:EDO:H11	1.69	0.56
1:B:149:ILE:HD11	4:B:1291:EDO:H11	1.86	0.56
1:B:181:ASP:HB3	1:B:184:THR:HG23	1.87	0.56
1:A:268:LYS:HG2	1:C:259:ASP:OD2	2.06	0.56
1:B:17:ARG:HH12	1:B:228:VAL:HG23	1.71	0.55
1:B:50:THR:HG21	1:B:54:ARG:HH21	1.73	0.54
1:B:252:SER:HB3	1:D:271:TYR:CE2	2.43	0.54
1:A:149:ILE:CD1	4:B:1291:EDO:H12	2.39	0.53
1:A:278:LYS:CB	1:C:275:THR:HG21	2.30	0.53
1:C:152:TYR:CE2	1:D:193:ILE:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:CG2	1:B:54:ARG:HH21	2.22	0.52
1:C:149:ILE:HD11	4:D:1292:EDO:C2	2.38	0.52
1:A:13:GLY:HA2	5:A:2058:HOH:O	2.09	0.52
1:A:193:ILE:HD11	1:B:152:TYR:CE2	2.46	0.51
1:B:286:THR:HB	1:C:288:ALA:HB2	1.91	0.50
1:C:140:THR:O	1:C:144:PHE:HB2	2.10	0.50
1:C:68:ASN:HA	1:C:85:LEU:HD22	1.94	0.50
1:B:97:TYR:CE2	1:B:161:ARG:CB	2.94	0.49
2:B:1289:NDP:H41N	3:B:1290:CB3:C7	2.41	0.49
1:A:156:LYS:HE3	1:B:136:MET:HE3	1.93	0.49
1:A:287:ARG:NH2	4:D:1291:EDO:O2	2.39	0.49
1:A:283:TYR:OH	3:A:1290:CB3:O	2.28	0.48
1:A:71:THR:HG23	1:A:88:ARG:NH1	2.28	0.48
1:A:140:THR:O	1:A:144:PHE:HB2	2.14	0.48
1:B:233:MET:HB2	1:B:234:PRO:HD2	1.96	0.48
1:B:140:THR:O	1:B:144:PHE:HB2	2.14	0.47
1:A:156:LYS:HE3	1:B:136:MET:CE	2.44	0.47
1:B:68:ASN:HA	1:B:85:LEU:HD22	1.96	0.47
2:D:1289:NDP:H41N	3:D:1290:CB3:C7	2.44	0.47
1:B:73:PRO:HG3	1:B:81:ALA:O	2.14	0.46
1:A:206:ARG:HH22	4:A:1292:EDO:C1	2.27	0.46
1:D:68:ASN:HD22	4:D:1292:EDO:C1	2.21	0.46
2:D:1289:NDP:H2D	3:D:1290:CB3:C2	2.45	0.46
1:A:275:THR:CG2	1:C:278:LYS:HB2	2.34	0.46
2:A:1289:NDP:H41N	3:A:1290:CB3:C7	2.46	0.45
1:D:140:THR:O	1:D:144:PHE:HB2	2.16	0.45
4:A:1293:EDO:O1	1:B:206:ARG:NE	2.39	0.45
1:D:151:PRO:O	1:D:155:ILE:HG13	2.17	0.45
1:D:168:LYS:HE2	1:D:169:HIS:CE1	2.52	0.45
1:C:193:ILE:HD11	1:D:152:TYR:CD2	2.51	0.45
1:A:17:ARG:NH1	1:A:228:VAL:HG23	2.32	0.44
1:B:258:SER:O	1:B:262:ILE:HD13	2.18	0.44
1:C:119:LEU:O	1:C:120:ARG:C	2.55	0.44
1:D:185:ASN:HB2	5:D:2017:HOH:O	2.18	0.44
4:A:1293:EDO:O1	1:B:203:GLY:HA2	2.18	0.44
1:C:16:LYS:HE3	1:C:40:SER:OG	2.18	0.44
1:C:181:ASP:HB3	1:C:184:THR:CG2	2.46	0.44
1:B:278:LYS:CB	1:D:275:THR:HG21	2.35	0.43
1:D:181:ASP:HB3	1:D:184:THR:CG2	2.46	0.43
1:B:71:THR:HG23	1:B:88:ARG:NH1	2.33	0.43
1:A:18:LEU:HD13	1:A:257:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG12	1:B:35:LEU:HD23	1.99	0.43
2:B:1289:NDP:H2D	3:B:1290:CB3:C2	2.48	0.43
1:C:149:ILE:CD1	4:D:1292:EDO:C2	2.84	0.43
1:A:193:ILE:HD11	1:B:152:TYR:CD2	2.54	0.43
1:D:68:ASN:HA	1:D:85:LEU:HD22	2.01	0.43
4:A:1293:EDO:H22	1:B:206:ARG:HH21	1.83	0.43
3:D:1290:CB3:C7	4:D:1291:EDO:H22	2.48	0.43
1:B:288:ALA:O	1:C:244:LYS:HD2	2.19	0.42
1:D:37:TYR:CE1	1:D:63:GLN:HG2	2.54	0.42
1:D:148:ALA:C	1:D:151:PRO:HD2	2.40	0.42
5:B:2039:HOH:O	3:C:1290:CB3:H13	2.19	0.42
1:A:152:TYR:CE2	1:B:193:ILE:HD11	2.55	0.42
1:B:233:MET:HG3	1:B:237:VAL:HB	2.01	0.42
1:A:68:ASN:HA	1:A:85:LEU:HD22	2.01	0.42
1:B:213:ALA:N	1:B:214:PRO:CD	2.82	0.42
1:D:36:HIS:CG	1:D:37:TYR:N	2.88	0.42
1:D:198:LYS:HD2	1:D:198:LYS:HA	1.90	0.42
1:A:37:TYR:O	1:A:63:GLN:HA	2.20	0.41
1:A:213:ALA:N	1:A:214:PRO:CD	2.82	0.41
3:D:1290:CB3:H13	4:D:1291:EDO:C2	2.51	0.41
1:D:38:HIS:HD2	1:D:63:GLN:NE2	2.18	0.41
1:C:38:HIS:HD2	1:C:63:GLN:NE2	2.19	0.41
1:A:38:HIS:HD2	1:A:63:GLN:NE2	2.19	0.41
1:C:160:HIS:HB2	1:D:120:ARG:NH1	2.36	0.41
1:D:213:ALA:N	1:D:214:PRO:CD	2.84	0.41
4:A:1293:EDO:C2	1:B:203:GLY:HA2	2.51	0.41
2:C:1289:NDP:H41N	3:C:1290:CB3:C7	2.51	0.41
1:B:228:VAL:O	1:B:228:VAL:CG2	2.65	0.41
1:C:72:ALA:O	1:C:73:PRO:C	2.58	0.40
1:A:227:SER:O	1:A:228:VAL:C	2.59	0.40
1:B:149:ILE:CD1	4:B:1291:EDO:C2	3.00	0.40
1:C:37:TYR:O	1:C:63:GLN:HA	2.21	0.40
1:A:152:TYR:CD2	1:B:193:ILE:HD11	2.57	0.40
1:A:238:TRP:CZ2	1:A:242:ARG:HD2	2.57	0.40
1:B:72:ALA:HA	1:B:73:PRO:HD3	1.80	0.40
1:B:213:ALA:HB3	1:B:214:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/288 (90%)	241 (93%)	17 (7%)	1 (0%)	34	60
1	B	260/288 (90%)	244 (94%)	14 (5%)	2 (1%)	19	43
1	C	245/288 (85%)	229 (94%)	15 (6%)	1 (0%)	34	60
1	D	247/288 (86%)	233 (94%)	12 (5%)	2 (1%)	19	43
All	All	1011/1152 (88%)	947 (94%)	58 (6%)	6 (1%)	25	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	B	180	VAL
1	C	180	VAL
1	D	180	VAL
1	B	228	VAL
1	D	228	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.