



Full wwPDB X-ray Structure Validation Report i

May 18, 2020 – 05:15 pm BST

PDB ID : 3GPR
Title : Crystal structure of rhodocetin
Authors : Stetefeld, J.
Deposited on : 2009-03-23
Resolution : 3.20 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 i symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

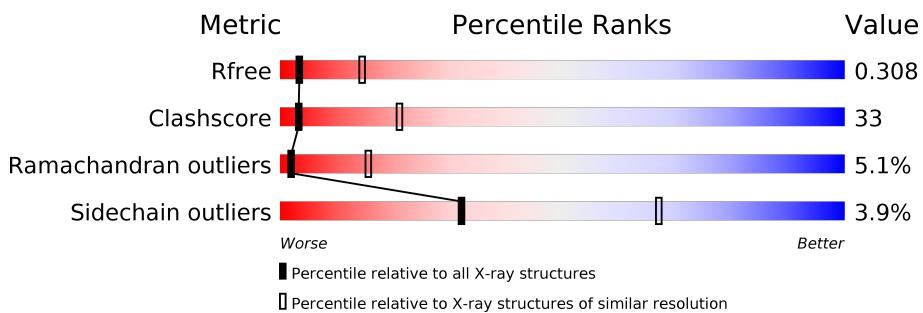
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain			
1	A	133	47%	47%	5%	: :
2	B	129	48%	47%
3	C	134	46%	47%	7%	
4	D	124	48%	46%	6%	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4295 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 Rhodocetin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1106	699	182	213	12	0	0	0

- Molecule 2 is a protein called Rhodocetin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	127	1055	686	177	186	6	0	0	0

- Molecule 3 is a protein called Rhodocetin subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	134	1096	687	192	207	10	0	0	0

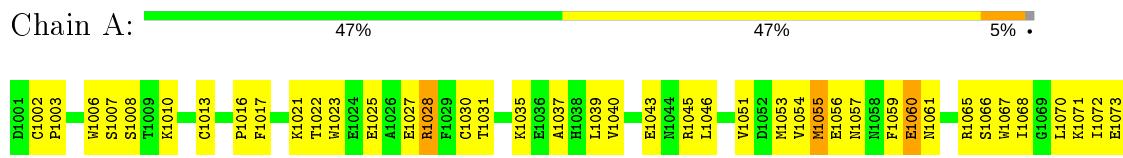
- Molecule 4 is a protein called Rhodocetin subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	124	1038	671	175	183	9	0	0	0

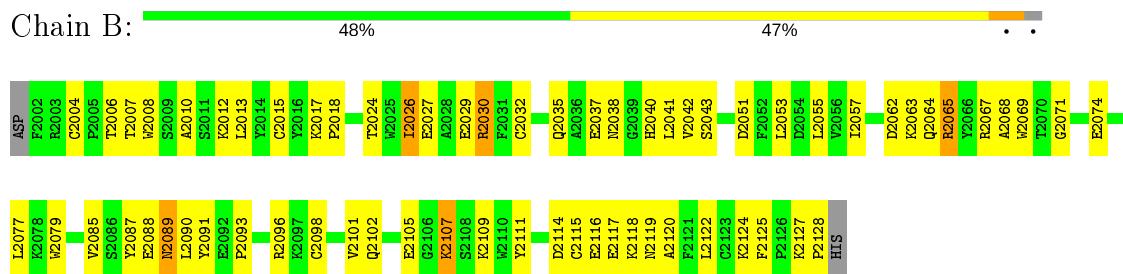
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

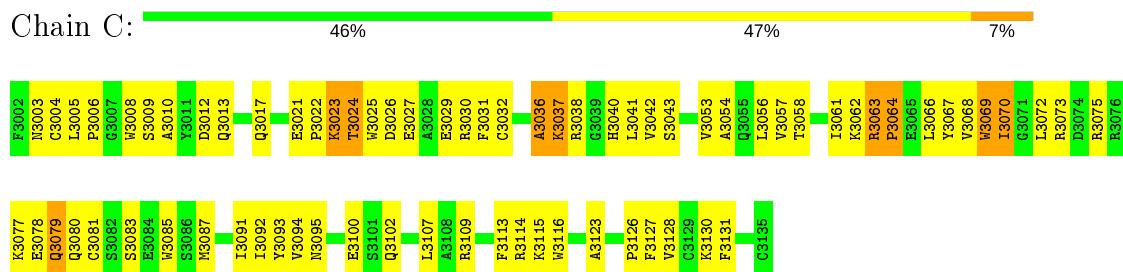
- Molecule 1: Rhodocetin subunit alpha



- Molecule 2: Rhodocetin subunit beta



- Molecule 3: Rhodocetin subunit gamma



- Molecule 4: Rhodocetin subunit delta





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	83.55 Å 83.55 Å 196.08 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.78 – 3.20 29.78 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.78-3.20) 99.9 (29.78-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	4.61 (at 3.31 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R , R_{free}	0.223 , 0.284 0.292 , 0.308	Depositor DCC
R_{free} test set	1207 reflections (10.37%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for -H-K, K, -L	Depositor
Outliers	0 of 11635 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	4295	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

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	0.26	0/1136	0.38	0/1528
2	B	0.27	0/1088	0.38	0/1471
3	C	0.27	0/1127	0.39	0/1523
4	D	0.27	0/1072	0.37	0/1449
All	All	0.27	0/4423	0.38	0/5971

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 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	1106	0	1028	76	0
2	B	1055	0	1024	66	0
3	C	1096	0	1007	98	0
4	D	1038	0	978	72	0
All	All	4295	0	4037	274	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 33.

All (274) 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:B:2030:ARG:HA	2:B:2030:ARG:HH11	1.31	0.96
1:A:1114:TRP:HB2	2:B:2090:LEU:HA	1.53	0.90
2:B:2069:TRP:HE1	2:B:2119:ASN:HB2	1.39	0.85
3:C:3070:ILE:HD13	3:C:3070:ILE:H	1.39	0.84
1:A:1111:LEU:HD12	1:A:1112:PRO:HD2	1.61	0.82
4:D:4110:ARG:HD3	4:D:4114:LYS:HD3	1.60	0.81
3:C:3068:VAL:HG23	3:C:3114:ARG:HH22	1.43	0.81
3:C:3066:LEU:HD21	3:C:3126:PRO:HG2	1.65	0.77
3:C:3116:TRP:HB2	4:D:4087:LYS:HA	1.67	0.76
1:A:1093:ASN:HD21	2:B:2109:LYS:HD3	1.52	0.75
3:C:3087:MET:HA	4:D:4037:ARG:HH21	1.50	0.74
1:A:1072:ILE:HD11	1:A:1101:LYS:HD2	1.69	0.74
3:C:3061:ILE:HD12	3:C:3063:ARG:H	1.49	0.74
1:A:1076:GLY:HA3	3:C:3078:GLU:HB2	1.68	0.74
3:C:3068:VAL:HG13	3:C:3127:PHE:HA	1.69	0.73
4:D:4075:LYS:HA	4:D:4081:ASP:HA	1.71	0.72
3:C:3057:VAL:HG12	3:C:3061:ILE:HG12	1.72	0.72
4:D:4019:LEU:HD23	4:D:4019:LEU:H	1.53	0.72
4:D:4030:TYR:HE2	4:D:4037:ARG:HG2	1.57	0.70
1:A:1083:TRP:HE1	1:A:1089:ILE:HG12	1.57	0.69
3:C:3058:THR:HB	3:C:3063:ARG:HG2	1.73	0.69
4:D:4070:ALA:HA	4:D:4093:ALA:HA	1.73	0.69
1:A:1068:ILE:HD11	1:A:1103:PHE:HB2	1.74	0.68
1:A:1072:ILE:HG22	2:B:2077:LEU:HD22	1.77	0.66
4:D:4015:VAL:HB	4:D:4057:THR:HG21	1.78	0.66
2:B:2069:TRP:NE1	2:B:2119:ASN:HB2	2.09	0.66
3:C:3037:LYS:HE2	3:C:3038:ARG:H	1.60	0.66
4:D:4076:TRP:HE1	4:D:4082:ALA:HA	1.60	0.66
3:C:3066:LEU:HD23	3:C:3067:TYR:N	2.10	0.66
3:C:3070:ILE:H	3:C:3070:ILE:CD1	2.08	0.66
4:D:4026:GLU:OE2	4:D:4038:LEU:HG	1.97	0.65
2:B:2063:LYS:O	2:B:2063:LYS:HD3	1.97	0.65
1:A:1107:HIS:HB2	1:A:1112:PRO:HB3	1.78	0.64
2:B:2107:LYS:N	2:B:2107:LYS:HE3	2.12	0.64
3:C:3037:LYS:CE	3:C:3038:ARG:H	2.11	0.63
3:C:3093:TYR:HB3	4:D:4042:HIS:HA	1.81	0.63
3:C:3040:HIS:ND1	4:D:4077:GLU:HG3	2.14	0.62
3:C:3025:TRP:CH2	3:C:3073:ARG:HB2	2.35	0.62
1:A:1065:ARG:HG2	1:A:1104:LEU:HD22	1.81	0.62
4:D:4065:LEU:HD13	4:D:4066:GLY:N	2.14	0.62
1:A:1085:ASP:HA	2:B:2040:HIS:ND1	2.15	0.61
3:C:3057:VAL:O	3:C:3061:ILE:HG13	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2053:LEU:HG	2:B:2057:ILE:HD11	1.83	0.61
1:A:1028:ARG:HB2	1:A:1028:ARG:NH2	2.14	0.61
3:C:3012:ASP:OD1	3:C:3013:GLN:HG3	2.01	0.61
1:A:1051:VAL:O	1:A:1055:MET:HB2	2.01	0.59
3:C:3027:GLU:O	3:C:3031:PHE:HB2	2.02	0.59
4:D:4084:LEU:HD23	4:D:4085:ASP:N	2.18	0.59
1:A:1016:PRO:HB3	1:A:1126:MET:HE3	1.86	0.58
3:C:3092:ILE:HD11	4:D:4042:HIS:HB2	1.86	0.58
4:D:4091:ARG:HG2	4:D:4094:TYR:CE1	2.39	0.58
3:C:3070:ILE:HG12	3:C:3072:LEU:HG	1.84	0.58
2:B:2127:LYS:HB2	2:B:2128:PRO:HD3	1.85	0.57
2:B:2042:VAL:HG21	2:B:2053:LEU:HD22	1.85	0.57
3:C:3095:ASN:HD22	4:D:4106:PHE:HA	1.69	0.57
2:B:2030:ARG:HH11	2:B:2030:ARG:CA	2.11	0.57
3:C:3061:ILE:HD12	3:C:3063:ARG:N	2.19	0.57
3:C:3070:ILE:HD13	3:C:3070:ILE:N	2.15	0.57
1:A:1027:GLU:OE2	1:A:1039:LEU:HG	2.05	0.57
2:B:2043:SER:HB3	2:B:2124:LYS:NZ	2.20	0.57
4:D:4065:LEU:HD12	4:D:4067:LEU:H	1.69	0.57
3:C:3032:CYS:SG	3:C:3041:LEU:HD23	2.45	0.56
1:A:1056:GLU:HB3	1:A:1061:ASN:HA	1.86	0.56
2:B:2102:GLN:HB2	2:B:2111:TYR:HE2	1.71	0.56
3:C:3024:THR:HA	3:C:3123:ALA:O	2.06	0.56
3:C:3037:LYS:HE2	3:C:3037:LYS:HA	1.86	0.56
2:B:2006:THR:O	2:B:2008:TRP:HD1	1.88	0.56
3:C:3061:ILE:O	3:C:3064:PRO:HD2	2.06	0.55
1:A:1068:ILE:HD11	1:A:1103:PHE:CB	2.36	0.55
2:B:2077:LEU:O	2:B:2085:VAL:HG23	2.06	0.55
4:D:4098:MET:HE3	4:D:4105:ILE:HG21	1.87	0.55
1:A:1065:ARG:HB3	1:A:1123:ASN:HD22	1.71	0.55
4:D:4067:LEU:HG	4:D:4069:ASN:ND2	2.21	0.55
2:B:2079:TRP:HE1	2:B:2085:VAL:HG22	1.72	0.55
2:B:2079:TRP:NE1	2:B:2085:VAL:HG22	2.22	0.55
3:C:3005:LEU:HB3	3:C:3006:PRO:HD2	1.89	0.55
1:A:1074:ASN:HD22	1:A:1074:ASN:H	1.56	0.54
3:C:3095:ASN:ND2	4:D:4106:PHE:HA	2.22	0.54
3:C:3037:LYS:HB3	3:C:3131:PHE:CD2	2.43	0.54
1:A:1065:ARG:HD3	1:A:1123:ASN:HD21	1.71	0.54
4:D:4036:SER:HA	4:D:4122:PHE:HB3	1.88	0.54
2:B:2030:ARG:HA	2:B:2030:ARG:NH1	2.12	0.54
1:A:1073:GLU:O	1:A:1079:SER:HA	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:LEU:HD23	1:A:1046:LEU:O	2.08	0.53
1:A:1023:TRP:CZ3	1:A:1071:LYS:HD2	2.43	0.53
3:C:3053:VAL:O	3:C:3057:VAL:HG23	2.07	0.53
1:A:1098:TYR:CD1	3:C:3094:VAL:HG23	2.43	0.53
2:B:2026:ILE:C	2:B:2026:ILE:HD13	2.29	0.53
2:B:2026:ILE:O	2:B:2026:ILE:HD13	2.08	0.53
3:C:3026:ASP:HB3	3:C:3030:ARG:HH12	1.73	0.53
3:C:3075:ARG:NH2	3:C:3080:GLN:HB2	2.24	0.53
1:A:1074:ASN:H	1:A:1074:ASN:ND2	2.07	0.52
1:A:1093:ASN:ND2	2:B:2109:LYS:HD3	2.21	0.52
1:A:1035:LYS:HD2	1:A:1129:PHE:HB2	1.91	0.52
2:B:2062:ASP:C	2:B:2064:GLN:H	2.12	0.52
3:C:3009:SER:HB2	3:C:3056:LEU:HD11	1.92	0.52
1:A:1098:TYR:N	1:A:1098:TYR:CD2	2.76	0.51
3:C:3029:GLU:CD	4:D:4077:GLU:HG2	2.31	0.51
3:C:3062:LYS:O	3:C:3063:ARG:HB2	2.09	0.51
3:C:3022:PRO:HB3	3:C:3126:PRO:HD3	1.93	0.51
3:C:3063:ARG:N	3:C:3064:PRO:CD	2.74	0.51
3:C:3094:VAL:HA	4:D:4107:TRP:CZ3	2.46	0.51
4:D:4021:THR:HA	4:D:4114:LYS:O	2.10	0.51
4:D:4003:LEU:O	4:D:4005:TRP:HD1	1.93	0.51
4:D:4071:TRP:H	4:D:4093:ALA:HA	1.76	0.51
2:B:2053:LEU:HD11	2:B:2122:LEU:HD13	1.93	0.50
2:B:2024:THR:OG1	2:B:2027:GLU:HG2	2.11	0.50
3:C:3005:LEU:HD11	3:C:3036:ALA:HB3	1.93	0.50
3:C:3017:GLN:C	3:C:3128:VAL:HG23	2.32	0.50
1:A:1054:VAL:HG12	1:A:1054:VAL:O	2.11	0.50
1:A:1121:GLU:HG2	1:A:1123:ASN:OD1	2.11	0.50
2:B:2067:ARG:HA	2:B:2101:VAL:O	2.12	0.50
4:D:4091:ARG:HD3	4:D:4091:ARG:C	2.32	0.50
1:A:1066:SER:OG	1:A:1125:PHE:HA	2.12	0.49
4:D:4065:LEU:HD12	4:D:4067:LEU:HB2	1.94	0.49
2:B:2088:GLU:OE1	2:B:2093:PRO:HA	2.11	0.49
1:A:1076:GLY:CA	3:C:3078:GLU:HB2	2.39	0.49
4:D:4019:LEU:CD2	4:D:4019:LEU:H	2.21	0.49
4:D:4075:LYS:HB2	4:D:4079:SER:O	2.13	0.49
1:A:1030:CYS:SG	1:A:1039:LEU:HD23	2.53	0.49
3:C:3042:VAL:HA	3:C:3130:LYS:HB2	1.95	0.49
3:C:3081:CYS:C	3:C:3083:SER:H	2.16	0.49
3:C:3029:GLU:HA	3:C:3041:LEU:HG	1.95	0.49
1:A:1075:LYS:CB	3:C:3077:LYS:HE2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2079:TRP:HE1	2:B:2085:VAL:HA	1.77	0.49
3:C:3037:LYS:HB3	3:C:3131:PHE:HD2	1.77	0.49
4:D:4116:VAL:HG12	4:D:4117:SER:N	2.27	0.49
1:A:1002:CYS:HB3	1:A:1006:TRP:HB2	1.95	0.49
1:A:1021:LYS:HB2	1:A:1125:PHE:HE2	1.77	0.49
1:A:1045:ARG:HA	2:B:2087:TYR:CE1	2.48	0.49
1:A:1084:SER:HB2	2:B:2029:GLU:OE1	2.13	0.49
1:A:1103:PHE:HD1	1:A:1103:PHE:H	1.61	0.49
3:C:3037:LYS:HE2	3:C:3038:ARG:N	2.27	0.49
3:C:3075:ARG:HB3	3:C:3102:GLN:HG3	1.94	0.49
4:D:4114:LYS:HG2	4:D:4115:THR:N	2.27	0.48
3:C:3068:VAL:HG11	3:C:3128:VAL:HG12	1.94	0.48
1:A:1080:ASN:N	1:A:1080:ASN:HD22	2.11	0.48
3:C:3113:PHE:HD1	3:C:3113:PHE:H	1.61	0.48
2:B:2102:GLN:HB2	2:B:2111:TYR:CE2	2.48	0.48
4:D:4063:MET:CE	4:D:4119:LEU:HD11	2.45	0.47
4:D:4012:CYS:HB2	4:D:4122:PHE:CE1	2.49	0.47
3:C:3004:CYS:SG	3:C:3010:ALA:HB2	2.55	0.47
1:A:1003:PRO:HB2	1:A:1006:TRP:CD1	2.50	0.47
1:A:1040:VAL:HG21	1:A:1051:VAL:HG11	1.96	0.47
2:B:2042:VAL:HG21	2:B:2053:LEU:CD2	2.43	0.47
3:C:3058:THR:HA	3:C:3061:ILE:HD11	1.97	0.47
1:A:1083:TRP:HA	2:B:2071:GLY:O	2.15	0.47
3:C:3058:THR:HA	3:C:3061:ILE:CD1	2.44	0.47
3:C:3085:TRP:HE1	3:C:3091:ILE:HD13	1.80	0.47
4:D:4084:LEU:C	4:D:4084:LEU:HD23	2.34	0.47
1:A:1060:GLU:N	1:A:1060:GLU:OE1	2.47	0.47
4:D:4102:THR:O	4:D:4102:THR:HG22	2.14	0.47
1:A:1074:ASN:HD22	1:A:1074:ASN:N	2.11	0.47
4:D:4030:TYR:CE2	4:D:4037:ARG:HG2	2.45	0.47
2:B:2004:CYS:SG	2:B:2010:ALA:HB2	2.55	0.46
2:B:2006:THR:HG22	2:B:2007:THR:N	2.30	0.46
4:D:4098:MET:HB3	4:D:4107:TRP:HD1	1.79	0.46
3:C:3021:GLU:O	3:C:3023:LYS:HD2	2.15	0.46
3:C:3075:ARG:HD3	3:C:3102:GLN:HE21	1.80	0.46
3:C:3042:VAL:HA	3:C:3130:LYS:CB	2.45	0.46
4:D:4019:LEU:HD23	4:D:4019:LEU:N	2.27	0.46
2:B:2062:ASP:CG	2:B:2063:LYS:H	2.18	0.46
1:A:1097:PRO:HB2	3:C:3093:TYR:CE1	2.51	0.46
1:A:1065:ARG:HD3	1:A:1123:ASN:ND2	2.31	0.46
1:A:1057:ASN:HA	1:A:1061:ASN:HD21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2018:PRO:HA	2:B:2122:LEU:HD23	1.97	0.46
3:C:3085:TRP:CZ3	4:D:4040:SER:HA	2.50	0.46
4:D:4065:LEU:CD1	4:D:4067:LEU:H	2.29	0.46
2:B:2051:ASP:O	2:B:2055:LEU:HG	2.16	0.46
4:D:4069:ASN:HB2	4:D:4094:TYR:O	2.16	0.46
3:C:3029:GLU:OE1	4:D:4077:GLU:HG2	2.16	0.46
2:B:2024:THR:HG23	2:B:2118:LYS:HG2	1.98	0.45
2:B:2114:ASP:C	2:B:2116:GLU:H	2.19	0.45
1:A:1031:THR:HG22	1:A:1037:ALA:O	2.16	0.45
4:D:4020:LYS:HB3	4:D:4024:ASP:OD1	2.16	0.45
4:D:4064:TRP:HH2	4:D:4114:LYS:HB3	1.80	0.45
3:C:3069:TRP:CE3	3:C:3069:TRP:HA	2.52	0.45
3:C:3109:ARG:NH2	3:C:3114:ARG:HD2	2.31	0.45
4:D:4096:ALA:HA	4:D:4108:TYR:O	2.17	0.45
2:B:2043:SER:HB3	2:B:2124:LYS:HZ1	1.82	0.45
4:D:4014:ARG:HG2	4:D:4015:VAL:N	2.32	0.45
2:B:2069:TRP:HE1	2:B:2119:ASN:HD22	1.65	0.45
1:A:1053:MET:C	1:A:1055:MET:H	2.20	0.45
2:B:2037:GLU:HG2	2:B:2038:ASN:ND2	2.32	0.45
2:B:2013:LEU:O	2:B:2127:LYS:HG3	2.17	0.45
1:A:1067:TRP:CE3	1:A:1104:LEU:HB3	2.51	0.45
1:A:1083:TRP:NE1	1:A:1089:ILE:HG12	2.30	0.45
3:C:3069:TRP:HA	3:C:3069:TRP:HE3	1.82	0.45
2:B:2069:TRP:HZ3	2:B:2098:CYS:HB2	1.82	0.44
2:B:2114:ASP:OD2	2:B:2116:GLU:HB2	2.16	0.44
3:C:3107:LEU:HD12	3:C:3115:LYS:O	2.17	0.44
4:D:4118:PHE:O	4:D:4119:LEU:HD23	2.16	0.44
4:D:4063:MET:HE1	4:D:4119:LEU:HD11	1.99	0.44
3:C:3077:LYS:NZ	3:C:3100:GLU:OE1	2.50	0.44
1:A:1114:TRP:NE1	2:B:2089:ASN:HB3	2.33	0.44
2:B:2067:ARG:HG2	2:B:2067:ARG:HH21	1.81	0.44
3:C:3080:GLN:O	3:C:3080:GLN:HG3	2.16	0.44
1:A:1105:MET:O	1:A:1105:MET:HG3	2.18	0.44
3:C:3094:VAL:HA	4:D:4107:TRP:HZ3	1.83	0.44
4:D:4064:TRP:CZ3	4:D:4110:ARG:HD2	2.53	0.43
1:A:1067:TRP:CZ3	1:A:1104:LEU:HD23	2.54	0.43
2:B:2032:CYS:SG	2:B:2041:LEU:HD23	2.58	0.43
4:D:4098:MET:HB3	4:D:4107:TRP:CD1	2.53	0.43
1:A:1035:LYS:C	1:A:1035:LYS:HD3	2.39	0.43
2:B:2068:ALA:O	2:B:2101:VAL:HG12	2.18	0.43
1:A:1080:ASN:O	2:B:2074:GLU:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3066:LEU:C	3:C:3066:LEU:HD23	2.38	0.43
4:D:4114:LYS:HG2	4:D:4115:THR:H	1.84	0.43
1:A:1007:SER:O	1:A:1013:CYS:HA	2.18	0.43
1:A:1055:MET:O	1:A:1059:PHE:HB2	2.19	0.43
2:B:2053:LEU:O	2:B:2057:ILE:HG13	2.19	0.43
3:C:3005:LEU:HB2	3:C:3008:TRP:CD1	2.54	0.43
3:C:3092:ILE:CG1	4:D:4042:HIS:HB2	2.49	0.43
1:A:1002:CYS:SG	1:A:1008:SER:HB3	2.58	0.43
3:C:3061:ILE:C	3:C:3061:ILE:HD12	2.39	0.43
3:C:3078:GLU:HG3	3:C:3079:GLN:N	2.34	0.43
3:C:3043:SER:HA	4:D:4076:TRP:CZ3	2.54	0.42
4:D:4067:LEU:CD2	4:D:4069:ASN:HD21	2.32	0.42
3:C:3083:SER:HA	4:D:4068:ASN:O	2.19	0.42
3:C:3087:MET:HA	4:D:4037:ARG:NH2	2.25	0.42
2:B:2035:GLN:NE2	2:B:2035:GLN:HA	2.35	0.42
3:C:3030:ARG:HH11	3:C:3030:ARG:HB2	1.84	0.42
3:C:3075:ARG:HH21	3:C:3078:GLU:HG2	1.84	0.42
2:B:2035:GLN:HE21	2:B:2035:GLN:HA	1.84	0.42
3:C:3067:TYR:HA	3:C:3107:LEU:O	2.19	0.42
4:D:4003:LEU:O	4:D:4004:HIS:HB2	2.20	0.42
4:D:4028:PHE:HD1	4:D:4118:PHE:HZ	1.68	0.42
1:A:1043:GLU:O	2:B:2087:TYR:HB2	2.19	0.42
4:D:4024:ASP:HA	4:D:4027:SER:OG	2.19	0.42
4:D:4024:ASP:O	4:D:4028:PHE:HB2	2.20	0.42
1:A:1046:LEU:C	1:A:1046:LEU:HD23	2.39	0.42
1:A:1059:PHE:O	1:A:1059:PHE:HD1	2.03	0.42
3:C:3078:GLU:C	3:C:3080:GLN:H	2.23	0.42
1:A:1016:PRO:HA	1:A:1126:MET:HA	2.03	0.41
2:B:2029:GLU:HA	2:B:2041:LEU:HG	2.02	0.41
2:B:2117:GLU:HG2	2:B:2119:ASN:ND2	2.35	0.41
3:C:3056:LEU:HD23	3:C:3056:LEU:C	2.40	0.41
4:D:4110:ARG:HG3	4:D:4110:ARG:HH21	1.84	0.41
1:A:1023:TRP:CH2	1:A:1071:LYS:HD2	2.54	0.41
2:B:2069:TRP:HD1	2:B:2120:ALA:O	2.04	0.41
2:B:2006:THR:O	2:B:2007:THR:HG22	2.21	0.41
3:C:3038:ARG:HH11	3:C:3038:ARG:HG2	1.86	0.41
1:A:1068:ILE:HD12	1:A:1070:LEU:HD12	2.01	0.41
1:A:1091:TYR:HA	3:C:3100:GLU:O	2.20	0.41
3:C:3061:ILE:HD12	3:C:3064:PRO:HD2	2.01	0.41
3:C:3116:TRP:HB2	4:D:4087:LYS:CA	2.43	0.41
3:C:3087:MET:CA	4:D:4037:ARG:HH21	2.25	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2026:ILE:O	2:B:2030:ARG:HG2	2.20	0.41
4:D:4067:LEU:HG	4:D:4069:ASN:HD21	1.84	0.41
2:B:2015:CYS:HB2	2:B:2125:PHE:CE1	2.56	0.41
3:C:3113:PHE:N	3:C:3113:PHE:CD1	2.89	0.41
1:A:1104:LEU:C	1:A:1104:LEU:HD12	2.42	0.41
3:C:3023:LYS:N	3:C:3023:LYS:HD2	2.36	0.41
1:A:1017:PHE:HD2	1:A:1125:PHE:HE1	1.69	0.41
2:B:2008:TRP:CD1	2:B:2017:LYS:HD2	2.56	0.41
2:B:2117:GLU:HG2	2:B:2119:ASN:HD21	1.86	0.41
4:D:4065:LEU:HD12	4:D:4067:LEU:CB	2.51	0.41
1:A:1065:ARG:CZ	1:A:1104:LEU:HD21	2.51	0.41
3:C:3025:TRP:HA	3:C:3069:TRP:CD1	2.56	0.41
1:A:1098:TYR:HD1	3:C:3094:VAL:HG23	1.85	0.41
4:D:4064:TRP:H2Z	4:D:4114:LYS:O	2.03	0.41
4:D:4031:ALA:O	4:D:4032:GLN:C	2.59	0.40
1:A:1022:THR:HG23	1:A:1025:GLU:H	1.86	0.40
1:A:1066:SER:HB2	1:A:1124:VAL:HG23	2.03	0.40
1:A:1068:ILE:HG22	1:A:1105:MET:HE2	2.03	0.40
2:B:2065:ARG:HG3	2:B:2065:ARG:O	2.21	0.40
3:C:3037:LYS:CA	3:C:3037:LYS:HE2	2.51	0.40
3:C:3063:ARG:N	3:C:3064:PRO:HD2	2.36	0.40
4:D:4069:ASN:N	4:D:4069:ASN:HD22	2.19	0.40
3:C:3054:ALA:HA	3:C:3109:ARG:HH21	1.86	0.40
1:A:1098:TYR:OH	3:C:3100:GLU:HG2	2.21	0.40
1:A:1114:TRP:N	1:A:1114:TRP:CD1	2.89	0.40
2:B:2026:ILE:HG23	2:B:2027:GLU:N	2.35	0.40
3:C:3092:ILE:CD1	4:D:4042:HIS:HB2	2.51	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	130/133 (98%)	103 (79%)	24 (18%)	3 (2%)	6 34
2	B	125/129 (97%)	91 (73%)	29 (23%)	5 (4%)	3 21
3	C	132/134 (98%)	92 (70%)	35 (26%)	5 (4%)	3 22
4	D	122/124 (98%)	84 (69%)	25 (20%)	13 (11%)	0 2
All	All	509/520 (98%)	370 (73%)	113 (22%)	26 (5%)	2 15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	3063	ARG
4	D	4104	ARG
2	B	2012	LYS
2	B	2065	ARG
2	B	2105	GLU
4	D	4032	GLN
4	D	4069	ASN
4	D	4071	TRP
4	D	4091	ARG
4	D	4103	ASP
1	A	1093	ASN
1	A	1103	PHE
2	B	2115	CYS
3	C	3003	ASN
3	C	3036	ALA
3	C	3064	PRO
4	D	4009	ASN
1	A	1010	LYS
2	B	2096	ARG
4	D	4078	TRP
4	D	4089	TRP
4	D	4117	SER
4	D	4064	TRP
4	D	4070	ALA
4	D	4097	VAL
3	C	3024	THR

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	123/124 (99%)	117 (95%)	6 (5%)	25 61
2	B	111/113 (98%)	106 (96%)	5 (4%)	27 63
3	C	117/117 (100%)	112 (96%)	5 (4%)	29 64
4	D	108/108 (100%)	106 (98%)	2 (2%)	57 81
All	All	459/462 (99%)	441 (96%)	18 (4%)	32 67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	ARG
1	A	1055	MET
1	A	1060	GLU
1	A	1074	ASN
1	A	1077	GLN
1	A	1080	ASN
2	B	2026	ILE
2	B	2030	ARG
2	B	2089	ASN
2	B	2091	TYR
2	B	2107	LYS
3	C	3023	LYS
3	C	3037	LYS
3	C	3069	TRP
3	C	3070	ILE
3	C	3079	GLN
4	D	4063	MET
4	D	4086	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1033	GLN
1	A	1061	ASN
1	A	1074	ASN
1	A	1080	ASN
1	A	1130	GLN
2	B	2035	GLN
2	B	2038	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2064	GLN
2	B	2089	ASN
2	B	2102	GLN
2	B	2119	ASN
3	C	3095	ASN
3	C	3102	GLN
3	C	3105	GLN
4	D	4069	ASN
4	D	4109	ASN

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 [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.