



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 3GPR / pdb_00003gpr
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

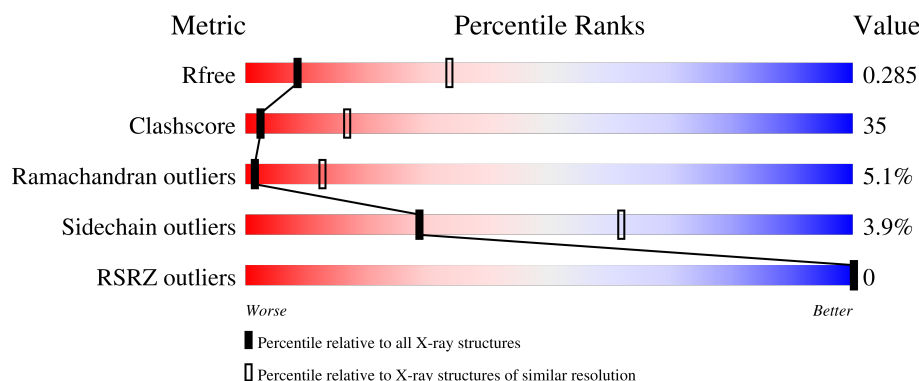
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

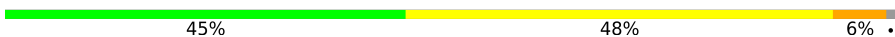
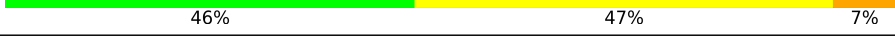
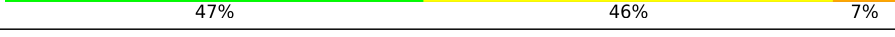
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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 $\leq 5\%$. 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	133	
2	B	129	
3	C	134	
4	D	124	

2 Entry composition

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
1	A	132	Total	C	N	O	S	0	0	0
			1106	699	182	213	12			

- Molecule 2 is a protein called Rhodocetin subunit beta.

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

- Molecule 3 is a protein called Rhodocetin subunit gamma.

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

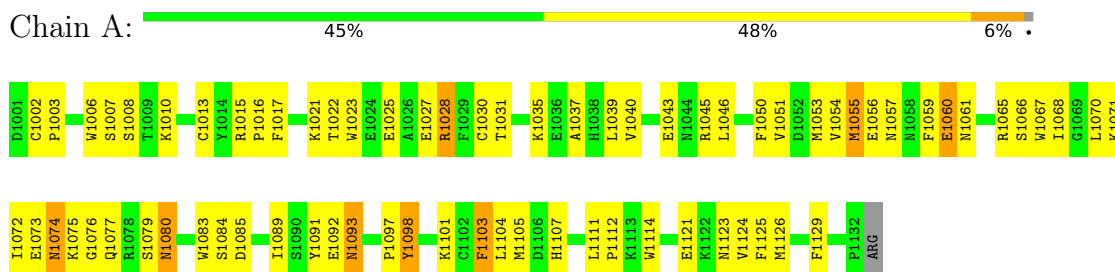
- Molecule 4 is a protein called Rhodocetin subunit delta.

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

3 Residue-property plots

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 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.

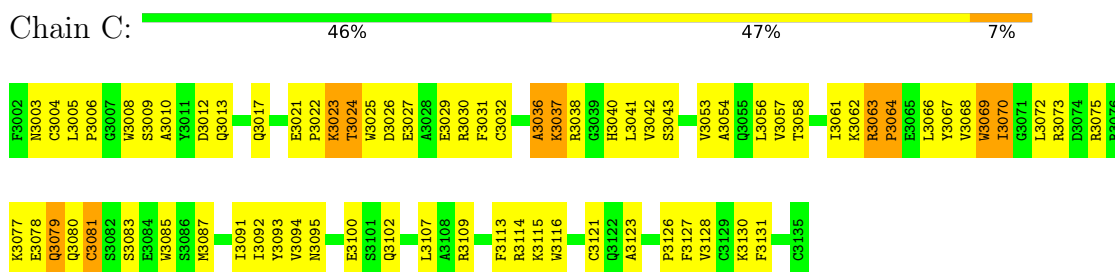
• Molecule 1: Rhodocetin subunit alpha



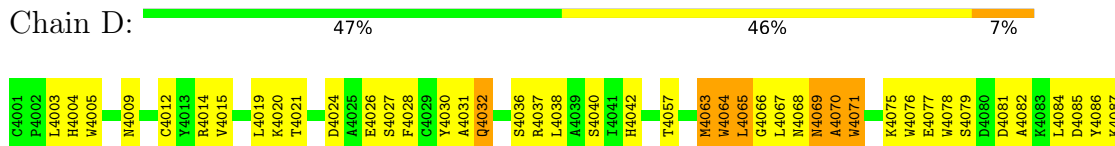
• Molecule 2: Rhodocetin subunit beta



• Molecule 3: Rhodocetin subunit gamma



• Molecule 4: Rhodocetin subunit delta



Y4088	Y4089	L4090	R4091	R4092	A4093	Y4094	C4095	A4096	Y4097	M4098		T4102	D4103	R4104	I4105	F4106	W4107	Y4108	M4109	R4110		K4114	T4115	W4116	S4117	F4118	L4119		F4122	Y4123	S4124
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	83.55Å 83.55Å 196.08Å 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 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.284 (Not available) , 0.285	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)	0.27 , 10.8	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	0.89	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

5.1 Standard geometry

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	0.25	0/1136	0.60	0/1528
2	B	0.27	0/1088	0.60	0/1471
3	C	0.27	0/1127	0.65	1/1523 (0.1%)
4	D	0.26	0/1072	0.58	0/1449
All	All	0.26	0/4423	0.61	1/5971 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3081	CYS	CB-CA-C	-5.21	110.14	117.23

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	1106	0	1028	83	0
2	B	1055	0	1024	70	0
3	C	1096	0	1007	102	0
4	D	1038	0	978	75	0
All	All	4295	0	4037	291	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 35.

All (291) 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:HH11	2:B:2030:ARG:HA	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:1016:PRO:HD3	1:A:1126:MET:HE2	1.66	0.75
4:D:4098:MET:HE3	4:D:4105:ILE:HG21	1.67	0.75
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
2:B:2043:SER:HB3	2:B:2124:LYS:HZ1	1.56	0.71
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:HE3	2:B:2107:LYS:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:D:4071:TRP:CD1	4:D:4092:ARG:HE	2.22	0.58
2:B:2026:ILE:HD13	2:B:2026:ILE:C	2.29	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
4:D:4065:LEU:HD12	4:D:4067:LEU:H	1.69	0.57
2:B:2043:SER:HB3	2:B:2124:LYS:NZ	2.20	0.56
2:B:2062:ASP:C	2:B:2064:GLN:H	2.12	0.56
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:3029:GLU:CD	4:D:4077:GLU:HG2	2.31	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
3:C:3017:GLN:C	3:C:3128:VAL:HG23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:4091:ARG:HD3	4:D:4091:ARG:C	2.32	0.54
3:C:3081:CYS:C	3:C:3083:SER:H	2.16	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
1:A:1023:TRP:CZ3	1:A:1071:LYS:HD2	2.43	0.53
1:A:1046:LEU:HD23	1:A:1046:LEU:O	2.08	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:HD13	2:B:2026:ILE:O	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
3:C:3009:SER:HB2	3:C:3056:LEU:HD11	1.92	0.52
4:D:4084:LEU:HD23	4:D:4084:LEU:C	2.34	0.51
1:A:1098:TYR:N	1:A:1098:TYR:CD2	2.76	0.51
2:B:2062:ASP:CG	2:B:2063:LYS:H	2.18	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
1:A:1054:VAL:O	1:A:1054:VAL:HG12	2.11	0.50
2:B:2114:ASP:C	2:B:2116:GLU:H	2.19	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
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
1:A:1053:MET:C	1:A:1055:MET:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	4:D:4019:LEU:CD2	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: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
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
1:A:1035:LYS:HD3	1:A:1035:LYS:C	2.39	0.48
3:C:3066:LEU:HD23	3:C:3066:LEU:C	2.38	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
3:C:3061:ILE:HD12	3:C:3061:ILE:C	2.39	0.47
4:D:4012:CYS:HB2	4:D:4122:PHE:CE1	2.49	0.47
4:D:4063:MET:CE	4:D:4119:LEU:HD11	2.45	0.47
3:C:3004:CYS:SG	3:C:3010:ALA:HB2	2.55	0.47
1:A:1050:PHE:HA	1:A:1053:MET:HE2	1.96	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:3056:LEU:HD23	3:C:3056:LEU:C	2.40	0.47
3:C:3058:THR:HA	3:C:3061:ILE:HD11	1.97	0.47
1:A:1046:LEU:HD23	1:A:1046:LEU:C	2.39	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
1:A:1060:GLU:N	1:A:1060:GLU:OE1	2.47	0.47
4:D:4102:THR:HG22	4:D:4102:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3042:VAL:HA	3:C:3130:LYS:CB	2.45	0.46
3:C:3075:ARG:HD3	3:C:3102:GLN:HE21	1.80	0.46
4:D:4019:LEU:HD23	4:D:4019:LEU:N	2.27	0.46
1:A:1097:PRO:HB2	3:C:3093:TYR:CE1	2.51	0.46
3:C:3078:GLU:C	3:C:3080:GLN:H	2.23	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
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
1:A:1006:TRP:NE1	1:A:1015:ARG:HH11	2.14	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
1:A:1031:THR:HG22	1:A:1037:ALA:O	2.16	0.45
1:A:1104:LEU:HD12	1:A:1104:LEU:C	2.42	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:HA	3:C:3069:TRP:CE3	2.52	0.45
3:C:3109:ARG:NH2	3:C:3114:ARG:HD2	2.31	0.45
4:D:4031:ALA:O	4:D:4032:GLN:C	2.59	0.45
4:D:4096:ALA:HA	4:D:4108:TYR:O	2.17	0.45
4:D:4014:ARG:HG2	4:D:4015:VAL:N	2.32	0.45
1:A:1055:MET:HE1	1:A:1059:PHE:HD2	1.82	0.45
2:B:2069:TRP:HE1	2:B:2119:ASN:HD22	1.65	0.45
2:B:2013:LEU:O	2:B:2127:LYS:HG3	2.17	0.45
2:B:2037:GLU:HG2	2:B:2038:ASN:ND2	2.32	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
3:C:3121:CYS:C	3:C:3123:ALA:H	2.26	0.44
2:B:2006:THR:HG22	2:B:2007:THR:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4118:PHE:O	4:D:4119:LEU:HD23	2.16	0.44
3:C:3077:LYS:NZ	3:C:3100:GLU:OE1	2.50	0.44
4:D:4063:MET:HE3	4:D:4119:LEU:HD11	2.00	0.44
1:A:1114:TRP:NE1	2:B:2089:ASN:HB3	2.33	0.44
2:B:2067:ARG:HH21	2:B:2067:ARG:HG2	1.81	0.44
3:C:3080:GLN:HG3	3:C:3080:GLN:O	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:1080:ASN:O	2:B:2074:GLU:HA	2.19	0.43
2:B:2063:LYS:HD3	2:B:2063:LYS:C	2.43	0.43
2:B:2068:ALA:O	2:B:2101:VAL:HG12	2.18	0.43
4:D:4114:LYS:HG2	4:D:4115:THR:H	1.84	0.43
3:C:3081:CYS:C	3:C:3083:SER:N	2.76	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: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
1:A:1092:GLU:C	3:C:3100:GLU:HB2	2.45	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
4:D:4003:LEU:C	4:D:4005:TRP:H	2.27	0.42
2:B:2035:GLN:HA	2:B:2035:GLN:HE21	1.84	0.42
2:B:2062:ASP:CG	2:B:2063:LYS:N	2.77	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:4005:TRP:NE1	4:D:4014:ARG:HH21	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4024:ASP:O	4:D:4028:PHE:HB2	2.20	0.42
1:A:1059:PHE:HD1	1:A:1059:PHE:O	2.03	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:3062:LYS:C	3:C:3064:PRO:HD3	2.44	0.41
4:D:4110:ARG:HH21	4:D:4110:ARG:HG3	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:2106:GLY:C	2:B:2107:LYS:HE3	2.45	0.41
2:B:2006:THR:O	2:B:2007:THR:HG22	2.21	0.41
2:B:2062:ASP:C	2:B:2064:GLN:N	2.79	0.41
3:C:3038:ARG:HG2	3:C:3038:ARG:HH11	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:3087:MET:CA	4:D:4037:ARG:HH21	2.25	0.41
3:C:3116:TRP:HB2	4:D:4087:LYS:CA	2.43	0.41
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:CD1	3:C:3113:PHE:N	2.89	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
3:C:3023:LYS:HD2	3:C:3023:LYS:N	2.36	0.41
4:D:4065:LEU:HD12	4:D:4067:LEU:CB	2.51	0.41
1:A:1053:MET:C	1:A:1055:MET:N	2.79	0.41
1:A:1065:ARG:CZ	1:A:1104:LEU:HD21	2.51	0.41
1:A:1098:TYR:HD1	3:C:3094:VAL:HG23	1.85	0.41
3:C:3025:TRP:HA	3:C:3069:TRP:CD1	2.56	0.41
4:D:4064:TRP:HZ2	4:D:4114:LYS:O	2.03	0.41
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
2:B:2065:ARG:HG3	2:B:2065:ARG:O	2.21	0.40
3:C:3037:LYS:HE2	3:C:3037:LYS:CA	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
1:A:1056:GLU:C	1:A:1061:ASN:HD22	2.29	0.40
1:A:1098:TYR:OH	3:C:3100:GLU:HG2	2.21	0.40
3:C:3054:ALA:HA	3:C:3109:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:TRP:O	1:A:1105:MET:HE3	2.20	0.40
1:A:1080:ASN:HD22	1:A:1080:ASN:C	2.29	0.40
1:A:1114:TRP:CD1	1:A:1114:TRP:N	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 [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	130/133 (98%)	103 (79%)	24 (18%)	3 (2%)	5	29
2	B	125/129 (97%)	91 (73%)	29 (23%)	5 (4%)	2	17
3	C	132/134 (98%)	92 (70%)	35 (26%)	5 (4%)	2	18
4	D	122/124 (98%)	84 (69%)	25 (20%)	13 (11%)	0	2
All	All	509/520 (98%)	370 (73%)	113 (22%)	26 (5%)	1	13

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	116 (94%)	7 (6%)	18	51
2	B	111/113 (98%)	108 (97%)	3 (3%)	39	68
3	C	117/117 (100%)	112 (96%)	5 (4%)	26	59
4	D	108/108 (100%)	105 (97%)	3 (3%)	38	68
All	All	459/462 (99%)	441 (96%)	18 (4%)	28	62

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

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Mol	Chain	Res	Type
1	A	1080	ASN
1	A	1098	TYR
2	B	2026	ILE
2	B	2030	ARG
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	4065	LEU
4	D	4086	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	1108	GLN
2	B	2035	GLN
2	B	2038	ASN
2	B	2064	GLN
2	B	2089	ASN
2	B	2102	GLN
2	B	2119	ASN
3	C	3035	GLN
3	C	3095	ASN
3	C	3102	GLN
3	C	3105	GLN
4	D	4069	ASN
4	D	4109	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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](#)

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	132/133 (99%)	-1.33	0 100 100	67, 123, 172, 178	0
2	B	127/129 (98%)	-1.46	0 100 100	54, 94, 118, 126	0
3	C	134/134 (100%)	-1.37	0 100 100	55, 115, 149, 153	0
4	D	124/124 (100%)	-1.47	0 100 100	20, 93, 111, 119	0
All	All	517/520 (99%)	-1.41	0 100 100	20, 101, 155, 178	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.