



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:19 pm BST

PDB ID : 2RH7
Title : Crystal Structures of the Luciferase and Green Fluorescent Protein from Renilla Reniformis
Authors : Loening, A.M.; Fenn, T.D.; Gambhir, S.S.
Deposited on : 2007-10-06
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

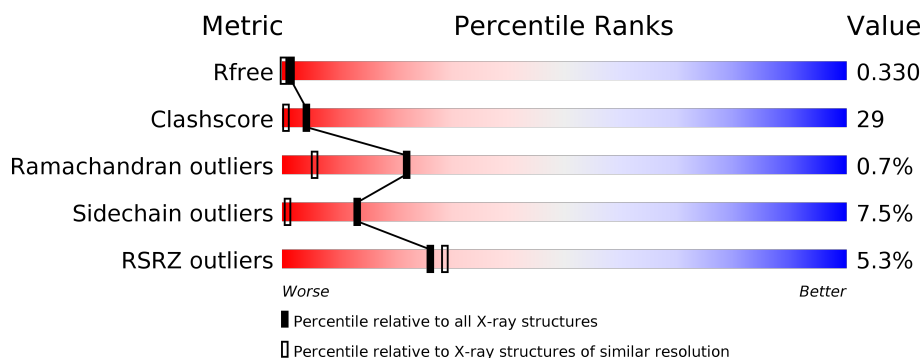
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 $\leq 5\%$. 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	239	<div> <div>4%</div> <div> <div>55%</div> <div>29%</div> <div>• • 11%</div> </div> </div>
1	B	239	<div> <div>5%</div> <div> <div>54%</div> <div>30%</div> <div>5% 11%</div> </div> </div>
1	C	239	<div> <div>5%</div> <div> <div>55%</div> <div>30%</div> <div>• 11%</div> </div> </div>
1	D	239	<div> <div>6%</div> <div> <div>52%</div> <div>31%</div> <div>5% 11%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CRO	A	66	-	-	X	-
1	CRO	B	66	-	-	X	-
1	CRO	C	66	-	-	X	-
1	CRO	D	66	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7391 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	3	0
			1714	1100	283	320	11			
1	B	213	Total	C	N	O	S	0	4	0
			1733	1110	285	329	9			
1	C	212	Total	C	N	O	S	0	1	0
			1700	1092	281	318	9			
1	D	212	Total	C	N	O	S	0	2	0
			1707	1097	283	317	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRO	SER	CHROMOPHORE	UNP Q963I9
A	66	CRO	TYR	CHROMOPHORE	UNP Q963I9
A	66	CRO	GLY	CHROMOPHORE	UNP Q963I9
A	234	VAL	-	EXPRESSION TAG	UNP Q963I9
A	235	ASP	-	EXPRESSION TAG	UNP Q963I9
A	236	HIS	-	EXPRESSION TAG	UNP Q963I9
A	237	HIS	-	EXPRESSION TAG	UNP Q963I9
A	238	HIS	-	EXPRESSION TAG	UNP Q963I9
A	239	HIS	-	EXPRESSION TAG	UNP Q963I9
A	240	HIS	-	EXPRESSION TAG	UNP Q963I9
A	241	HIS	-	EXPRESSION TAG	UNP Q963I9
B	66	CRO	SER	CHROMOPHORE	UNP Q963I9
B	66	CRO	TYR	CHROMOPHORE	UNP Q963I9
B	66	CRO	GLY	CHROMOPHORE	UNP Q963I9
B	234	VAL	-	EXPRESSION TAG	UNP Q963I9
B	235	ASP	-	EXPRESSION TAG	UNP Q963I9
B	236	HIS	-	EXPRESSION TAG	UNP Q963I9
B	237	HIS	-	EXPRESSION TAG	UNP Q963I9
B	238	HIS	-	EXPRESSION TAG	UNP Q963I9
B	239	HIS	-	EXPRESSION TAG	UNP Q963I9
B	240	HIS	-	EXPRESSION TAG	UNP Q963I9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	HIS	-	EXPRESSION TAG	UNP Q963I9
C	66	CRO	SER	CHROMOPHORE	UNP Q963I9
C	66	CRO	TYR	CHROMOPHORE	UNP Q963I9
C	66	CRO	GLY	CHROMOPHORE	UNP Q963I9
C	234	VAL	-	EXPRESSION TAG	UNP Q963I9
C	235	ASP	-	EXPRESSION TAG	UNP Q963I9
C	236	HIS	-	EXPRESSION TAG	UNP Q963I9
C	237	HIS	-	EXPRESSION TAG	UNP Q963I9
C	238	HIS	-	EXPRESSION TAG	UNP Q963I9
C	239	HIS	-	EXPRESSION TAG	UNP Q963I9
C	240	HIS	-	EXPRESSION TAG	UNP Q963I9
C	241	HIS	-	EXPRESSION TAG	UNP Q963I9
D	66	CRO	SER	CHROMOPHORE	UNP Q963I9
D	66	CRO	TYR	CHROMOPHORE	UNP Q963I9
D	66	CRO	GLY	CHROMOPHORE	UNP Q963I9
D	234	VAL	-	EXPRESSION TAG	UNP Q963I9
D	235	ASP	-	EXPRESSION TAG	UNP Q963I9
D	236	HIS	-	EXPRESSION TAG	UNP Q963I9
D	237	HIS	-	EXPRESSION TAG	UNP Q963I9
D	238	HIS	-	EXPRESSION TAG	UNP Q963I9
D	239	HIS	-	EXPRESSION TAG	UNP Q963I9
D	240	HIS	-	EXPRESSION TAG	UNP Q963I9
D	241	HIS	-	EXPRESSION TAG	UNP Q963I9

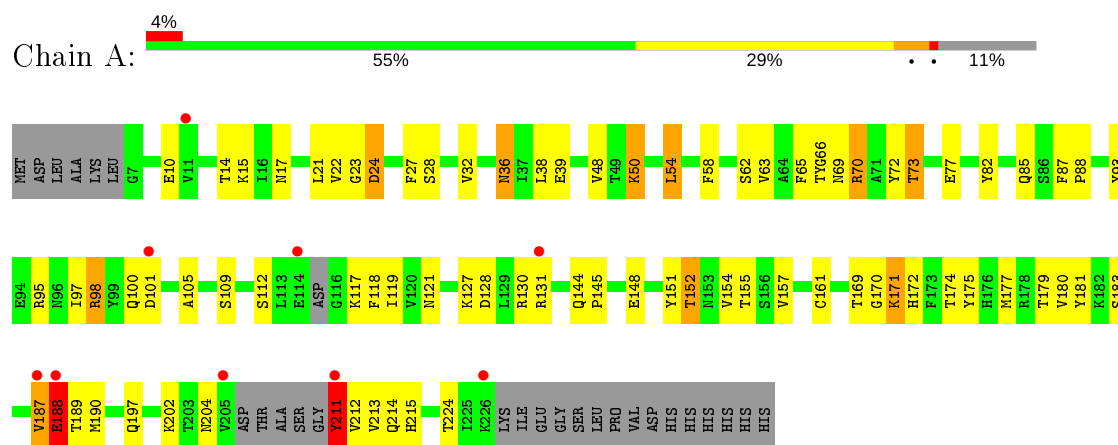
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 132 132	0	0
2	B	138	Total O 138 138	0	0
2	C	146	Total O 146 146	0	0
2	D	121	Total O 121 121	0	0

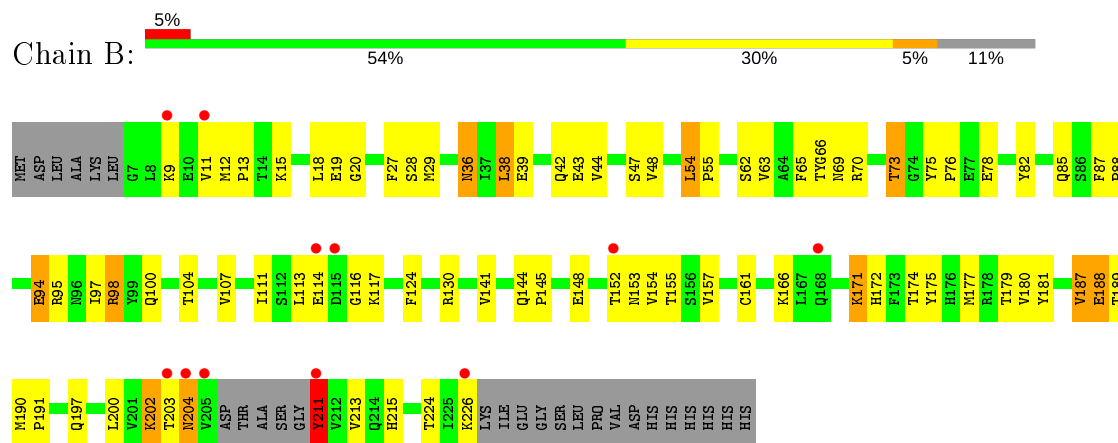
3 Residue-property plots [i](#)

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

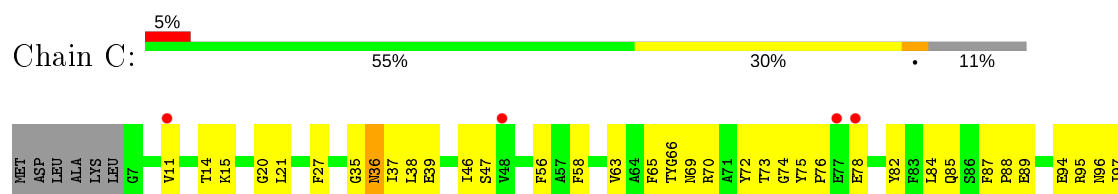
• Molecule 1: Green fluorescent protein

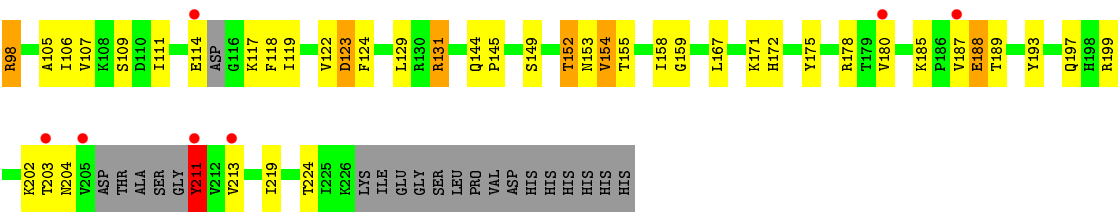


• Molecule 1: Green fluorescent protein

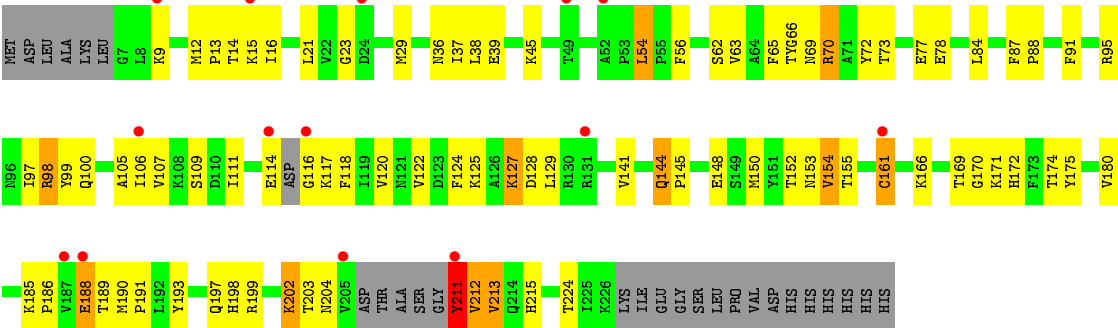


• Molecule 1: Green fluorescent protein





● Molecule 1: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	73.74Å 85.41Å 158.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 45.63 – 1.50	Depositor EDS
% Data completeness (in resolution range)	76.8 (50.00-1.50) 86.7 (45.63-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.291 , 0.325 0.301 , 0.330	Depositor DCC
R_{free} test set	7018 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 88.59 % 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 4.6402e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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

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	0/1728	0.62	1/2330 (0.0%)
1	B	0.40	0/1748	0.61	1/2359 (0.0%)
1	C	0.39	0/1714	0.61	1/2311 (0.0%)
1	D	0.38	0/1722	0.62	1/2322 (0.0%)
All	All	0.39	0/6912	0.62	4/9322 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	211	TYR	N-CA-C	-8.21	88.84	111.00
1	A	211	TYR	N-CA-C	-7.08	91.87	111.00
1	B	211	TYR	N-CA-C	-6.45	93.59	111.00
1	D	211	TYR	N-CA-C	-5.87	95.14	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	TYR	Peptide
1	B	211	TYR	Peptide
1	C	211	TYR	Peptide
1	D	211	TYR	Peptide

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	1714	0	1689	93	0
1	B	1733	0	1698	124	0
1	C	1700	0	1676	91	0
1	D	1707	0	1689	117	0
2	A	132	0	0	11	0
2	B	138	0	0	16	0
2	C	146	0	0	10	0
2	D	121	0	0	9	0
All	All	7391	0	6752	398	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 29.

All (398) 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:A:70:ARG:HH11	1:A:70:ARG:HG2	1.04	1.17
1:C:14:THR:HG22	1:C:118:PHE:HB2	1.33	1.10
1:A:14:THR:HG22	1:A:118:PHE:HB2	1.20	1.09
1:D:14:THR:HG22	1:D:118:PHE:HB2	1.28	1.07
1:D:152:THR:HG21	1:D:190:MET:HB3	1.36	1.02
1:A:48:VAL:HG21	1:A:54:LEU:HD11	1.43	1.00
1:B:48:VAL:HG21	1:B:54:LEU:HD11	1.43	1.00
1:A:65:PHE:C	1:A:66:CRO:N1	2.18	0.97
1:D:63:VAL:HG12	1:D:95:ARG:NH1	1.79	0.96
1:D:66:CRO:HB2	1:D:70:ARG:HH22	1.31	0.95
1:A:224:THR:H	1:B:197:GLN:HE22	1.16	0.93
1:A:66:CRO:C3	1:A:69:ASN:N	2.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:NZ	1:B:172:HIS:H	1.66	0.92
1:C:224:THR:H	1:D:197:GLN:HE22	1.13	0.91
1:C:70:ARG:HE	1:C:73:THR:CG2	1.82	0.91
1:C:180:VAL:HB	2:C:324:HOH:O	1.68	0.91
1:C:153:ASN:HA	1:D:171:LYS:HE2	1.51	0.91
1:B:171:LYS:HG3	1:B:172:HIS:N	1.84	0.90
1:A:169:THR:HB	1:C:188:GLU:HG2	1.54	0.90
1:B:66:CRO:C3	1:B:69:ASN:N	2.36	0.89
1:C:65:PHE:C	1:C:66:CRO:N1	2.26	0.89
1:B:85:GLN:HG2	2:B:318:HOH:O	1.73	0.88
1:D:36:ASN:HD22	1:D:39:GLU:H	1.16	0.88
1:C:66:CRO:C3	1:C:69:ASN:N	2.36	0.87
1:C:70:ARG:HE	1:C:73:THR:HG21	1.39	0.86
1:A:54:LEU:HD12	1:A:54:LEU:H	1.40	0.86
1:B:65:PHE:C	1:B:66:CRO:N1	2.29	0.86
1:D:62:SER:O	1:D:66:CRO:N1	2.08	0.85
1:D:66:CRO:C3	1:D:69:ASN:N	2.38	0.85
1:D:65:PHE:C	1:D:66:CRO:N1	2.29	0.85
1:D:98:ARG:HD3	1:D:98:ARG:N	1.91	0.85
1:D:180:VAL:HB	2:D:358:HOH:O	1.77	0.84
1:C:197:GLN:HE22	1:D:224:THR:H	1.26	0.84
1:C:63:VAL:HG12	1:C:95:ARG:NH1	1.93	0.83
1:B:70:ARG:O	1:B:73:THR:HG23	1.79	0.83
1:D:66:CRO:HA31	1:D:69:ASN:N	1.94	0.83
1:B:82:TYR:CE1	1:B:187:VAL:HG11	2.14	0.82
1:B:66:CRO:CA3	1:B:69:ASN:N	2.42	0.82
1:B:171:LYS:HZ2	1:B:172:HIS:H	1.26	0.82
1:C:66:CRO:CA3	1:C:69:ASN:N	2.44	0.81
1:A:10:GLU:HG3	1:A:38:LEU:HD22	1.63	0.81
1:D:66:CRO:CA3	1:D:69:ASN:N	2.44	0.80
1:A:66:CRO:CA3	1:A:69:ASN:N	2.45	0.80
1:B:70:ARG:HE	1:B:73:THR:HG21	1.45	0.80
1:A:70:ARG:HH11	1:A:70:ARG:CG	1.91	0.80
1:A:70:ARG:NH1	1:A:70:ARG:HG2	1.84	0.79
1:A:54:LEU:HD12	1:A:54:LEU:N	1.96	0.79
1:A:65:PHE:C	1:A:66:CRO:H2	1.82	0.79
1:B:189:THR:HG21	1:D:170:GLY:HA3	1.65	0.78
1:A:152:THR:HG22	2:A:251:HOH:O	1.83	0.78
1:B:188:GLU:CD	1:B:188:GLU:H	1.87	0.78
1:A:15:LYS:HG2	1:A:117:LYS:HD2	1.66	0.77
1:D:152:THR:CG2	1:D:190:MET:HB3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:O	1:A:73:THR:HG23	1.86	0.76
1:C:89:GLU:OE1	1:C:185:LYS:HD3	1.86	0.75
1:C:193:TYR:CD2	1:D:144:GLN:HG2	2.22	0.75
1:C:66:CRO:HA31	1:C:69:ASN:N	2.02	0.74
1:A:48:VAL:CG2	1:A:54:LEU:HD11	2.17	0.74
1:B:66:CRO:HA31	1:B:69:ASN:N	2.03	0.74
1:B:70:ARG:HE	1:B:73:THR:CG2	2.00	0.74
1:A:171:LYS:HG3	1:A:172:HIS:N	2.02	0.73
1:C:14:THR:HG23	1:C:72:TYR:OH	1.87	0.73
1:D:148:GLU:HA	1:D:161[A]:CYS:HB2	1.69	0.73
1:C:145:PRO:HG3	1:C:199:ARG:HG3	1.71	0.72
1:D:36:ASN:ND2	1:D:39:GLU:H	1.87	0.72
1:A:204:ASN:HB3	1:A:213:VAL:HG12	1.72	0.72
1:B:175:TYR:HE2	1:B:177:MET:CE	2.03	0.72
1:A:97:ILE:HG23	1:A:175:TYR:CD2	2.25	0.71
1:D:109:SER:HB2	1:D:122:VAL:HG13	1.70	0.71
1:A:197:GLN:HE22	1:B:224:THR:H	1.38	0.71
1:D:14:THR:HG23	1:D:72:TYR:OH	1.91	0.71
1:B:204:ASN:HB3	1:B:213:VAL:CG1	2.20	0.70
1:B:152[B]:THR:CG2	1:B:191:PRO:HD2	2.21	0.70
1:A:98:ARG:HD2	2:A:263:HOH:O	1.90	0.70
1:D:171:LYS:NZ	1:D:172:HIS:H	1.90	0.70
1:D:114:GLU:H	1:D:116:GLY:HA2	1.57	0.70
1:A:62:SER:HB2	1:A:214:GLN:HE22	1.56	0.69
1:B:204:ASN:HB3	1:B:213:VAL:HG12	1.72	0.69
1:B:152[B]:THR:HG21	1:B:190:MET:HB3	1.75	0.69
1:C:171:LYS:HE2	1:D:153:ASN:HA	1.74	0.69
1:A:50:LYS:HZ2	1:A:50:LYS:HB2	1.58	0.69
1:B:189:THR:HG22	2:C:263:HOH:O	1.92	0.69
1:D:215:HIS:HD2	2:D:257:HOH:O	1.76	0.68
1:C:15:LYS:HG2	1:C:117:LYS:HD2	1.74	0.68
1:A:54:LEU:CD1	1:A:54:LEU:H	2.06	0.68
1:D:70:ARG:HD3	2:D:259:HOH:O	1.92	0.68
1:B:36:ASN:ND2	1:B:38:LEU:H	1.91	0.68
1:B:36:ASN:HD22	1:B:38:LEU:H	1.41	0.68
1:D:109:SER:OG	1:D:122:VAL:HG22	1.92	0.68
1:A:66:CRO:HA31	1:A:69:ASN:N	2.08	0.67
1:B:226:LYS:HB3	2:B:361:HOH:O	1.94	0.67
1:B:15:LYS:NZ	1:B:117:LYS:HD2	2.09	0.67
1:D:141:VAL:HB	1:D:166[A]:LYS:HG3	1.77	0.67
1:B:152[B]:THR:HG22	1:B:191:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:OE1	1:D:189:THR:HG22	1.94	0.67
1:A:62:SER:CB	1:A:214:GLN:HE22	2.08	0.66
1:C:85:GLN:HE21	1:C:187:VAL:CG2	2.09	0.66
1:B:63:VAL:HG12	1:B:95:ARG:NH1	2.10	0.66
1:D:105:ALA:HB1	2:D:350:HOH:O	1.94	0.66
1:A:66:CRO:O3	1:A:69:ASN:N	2.28	0.66
1:B:215:HIS:HD2	2:B:250:HOH:O	1.78	0.65
1:B:85:GLN:NE2	1:B:187:VAL:HG23	2.11	0.65
1:C:171:LYS:NZ	1:C:172:HIS:H	1.94	0.65
1:B:100:GLN:NE2	1:B:174:THR:H	1.94	0.65
1:C:204:ASN:HB3	1:C:213:VAL:HG12	1.78	0.65
1:D:100:GLN:HE21	1:D:174:THR:H	1.45	0.65
1:A:50:LYS:NZ	1:A:50:LYS:HB2	2.11	0.65
1:B:98:ARG:HG3	1:B:104:THR:HG22	1.77	0.65
1:C:224:THR:N	1:D:197:GLN:HE22	1.92	0.65
1:A:82:TYR:HE1	1:A:187:VAL:HG11	1.61	0.64
1:B:65:PHE:C	1:B:66:CRO:H2	1.97	0.64
1:B:148:GLU:HA	1:B:161:CYS:HB3	1.80	0.64
1:A:14:THR:HG23	1:A:72:TYR:OH	1.97	0.64
1:B:177:MET:SD	2:B:379:HOH:O	2.55	0.64
1:C:63:VAL:HG13	1:C:66:CRO:CB2	2.27	0.63
1:C:152:THR:HG22	2:C:343:HOH:O	1.97	0.63
1:D:106:ILE:O	1:D:106:ILE:HG13	1.98	0.63
1:D:152:THR:CG2	1:D:191:PRO:HD2	2.28	0.63
1:D:70:ARG:HG3	1:D:73:THR:HG21	1.78	0.63
1:D:66:CRO:HB2	1:D:70:ARG:NH2	2.11	0.63
1:A:204:ASN:HB3	1:A:213:VAL:CG1	2.29	0.63
1:C:70:ARG:NE	1:C:73:THR:CG2	2.60	0.63
1:D:152:THR:HG22	1:D:191:PRO:HD2	1.80	0.63
1:C:153:ASN:CA	1:D:171:LYS:HE2	2.26	0.63
1:B:157:VAL:CG1	1:B:181:TYR:HB2	2.29	0.62
1:B:175:TYR:HE2	1:B:177:MET:HE3	1.63	0.62
1:B:94:GLU:HG2	2:B:301:HOH:O	1.99	0.62
1:D:114:GLU:N	1:D:116:GLY:HA2	2.11	0.62
1:B:175:TYR:CE2	1:B:177:MET:CE	2.83	0.62
1:B:11:VAL:HG22	2:B:285:HOH:O	1.99	0.61
1:D:152:THR:HG21	1:D:190:MET:CB	2.24	0.61
1:C:144:GLN:HG3	1:C:145:PRO:HD2	1.82	0.61
1:B:18:LEU:HD22	1:B:29:MET:HE3	1.82	0.61
1:B:54:LEU:HD12	1:B:54:LEU:N	2.15	0.60
1:A:14:THR:HG22	1:A:118:PHE:CB	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PHE:C	1:D:66:CRO:CA1	2.70	0.59
1:C:111:ILE:HD12	1:C:111:ILE:N	2.17	0.59
1:A:117:LYS:HE3	1:A:119:ILE:HD11	1.83	0.59
1:A:157:VAL:HG13	1:A:181:TYR:HB2	1.84	0.59
1:B:157:VAL:HG13	1:B:181:TYR:HB2	1.84	0.59
1:B:47:SER:HB2	1:B:211:TYR:HE1	1.68	0.59
1:D:100:GLN:NE2	1:D:174:THR:H	2.00	0.59
1:D:204:ASN:HB3	1:D:213:VAL:HG13	1.83	0.59
1:A:171:LYS:HE2	2:A:361:HOH:O	2.02	0.59
1:A:65:PHE:O	1:A:66:CRO:N1	2.36	0.59
1:C:144:GLN:HG2	1:D:193:TYR:CD2	2.38	0.58
1:A:15:LYS:HE2	1:A:117:LYS:HZ2	1.68	0.58
1:B:15:LYS:HB3	2:B:369:HOH:O	2.02	0.58
1:A:171:LYS:HE3	1:A:172:HIS:O	2.03	0.57
1:D:127:LYS:NZ	1:D:128:ASP:H	2.02	0.57
1:B:9:LYS:HG2	2:B:285:HOH:O	2.03	0.57
1:B:171:LYS:CG	1:B:172:HIS:N	2.62	0.57
1:A:63:VAL:HG11	1:A:177:MET:SD	2.44	0.57
1:A:180:VAL:HG13	2:A:289:HOH:O	2.04	0.57
1:A:87:PHE:HB3	1:A:88:PRO:HA	1.87	0.57
1:B:175:TYR:CE2	1:B:177:MET:HE3	2.39	0.57
1:B:69:ASN:N	2:B:251:HOH:O	2.38	0.57
1:C:96:ASN:ND2	1:C:106:ILE:HD12	2.20	0.57
1:D:98:ARG:CD	1:D:98:ARG:N	2.65	0.57
1:C:171:LYS:HE2	1:D:153:ASN:CA	2.35	0.56
1:D:148:GLU:HA	1:D:161[B]:CYS:HB3	1.87	0.56
1:C:171:LYS:HE2	1:D:153:ASN:CB	2.35	0.56
2:C:325:HOH:O	1:D:199:ARG:HD2	2.05	0.56
1:C:82:TYR:CE1	1:C:187:VAL:HG11	2.40	0.56
1:D:9:LYS:O	1:D:12:MET:HG2	2.06	0.56
1:B:155:THR:O	1:B:155:THR:HG22	2.05	0.56
1:C:36:ASN:HD22	1:C:38:LEU:H	1.53	0.56
1:C:82:TYR:CD1	1:C:187:VAL:HG11	2.41	0.56
1:B:171:LYS:NZ	1:B:172:HIS:N	2.48	0.56
1:A:151:TYR:HD2	1:B:171:LYS:HZ1	1.55	0.55
1:D:66:CRO:CB2	1:D:70:ARG:HH12	2.20	0.55
1:C:70:ARG:NE	1:C:73:THR:HG21	2.16	0.55
1:D:171:LYS:HZ3	1:D:172:HIS:H	1.55	0.55
1:C:87:PHE:HB3	1:C:88:PRO:HA	1.89	0.55
1:A:101[B]:ASP:OD2	1:A:130:ARG:HG2	2.07	0.55
1:D:78:GLU:CD	1:D:78:GLU:N	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CE1	1:A:187:VAL:HG11	2.41	0.55
1:B:27:PHE:HE1	1:B:29:MET:HE2	1.72	0.55
1:D:37:ILE:HG13	1:D:38:LEU:HD13	1.89	0.55
1:A:215:HIS:HD2	2:A:293:HOH:O	1.90	0.54
1:B:175:TYR:HE2	1:B:177:MET:HE2	1.70	0.54
1:B:70:ARG:NE	1:B:70:ARG:HA	2.21	0.54
1:C:152:THR:CG2	2:C:267:HOH:O	2.54	0.54
1:D:127:LYS:HZ1	1:D:128:ASP:H	1.55	0.54
1:B:15:LYS:HZ2	1:B:117:LYS:HD2	1.71	0.54
1:B:70:ARG:O	1:B:73:THR:CG2	2.53	0.54
1:C:109:SER:OG	1:C:122:VAL:HG22	2.07	0.54
1:A:105:ALA:HB1	2:A:339:HOH:O	2.07	0.54
1:D:145:PRO:HG3	1:D:199:ARG:HG3	1.89	0.54
1:A:14:THR:HG21	2:A:265:HOH:O	2.08	0.53
1:D:144:GLN:HG3	1:D:145:PRO:HD2	1.90	0.53
1:B:100:GLN:HE21	1:B:174:THR:H	1.56	0.53
1:B:175:TYR:CE2	1:B:177:MET:HE2	2.44	0.53
1:A:188:GLU:N	1:A:188:GLU:OE1	2.41	0.53
1:C:70:ARG:HH21	1:C:73:THR:HG22	1.74	0.53
1:A:23:GLY:HA2	1:A:127:LYS:HD2	1.89	0.53
1:A:183:SER:HB3	2:A:337:HOH:O	2.08	0.53
1:C:94:GLU:HB2	1:C:180:VAL:CG1	2.39	0.53
1:C:74:GLY:O	1:C:219:ILE:HD12	2.09	0.53
1:A:169:THR:CB	1:C:188:GLU:HG2	2.33	0.52
1:D:65:PHE:C	1:D:66:CRO:H2	2.11	0.52
1:A:171:LYS:HE3	1:A:172:HIS:H	1.74	0.52
1:C:203:THR:OG1	1:C:213:VAL:HG13	2.09	0.52
1:C:144:GLN:HG2	1:D:193:TYR:CG	2.44	0.52
1:C:171:LYS:HE2	1:D:153:ASN:HB2	1.92	0.52
1:B:189:THR:HG23	1:D:169:THR:O	2.10	0.52
1:C:204:ASN:HB3	1:C:213:VAL:CG1	2.39	0.52
1:B:97:ILE:CD1	1:B:177:MET:HE2	2.40	0.52
1:C:46:ILE:HD12	1:C:58:PHE:HZ	1.74	0.52
1:A:155:THR:O	1:A:155:THR:HG22	2.09	0.52
1:B:63:VAL:HG11	1:B:177:MET:SD	2.49	0.52
1:C:65:PHE:C	1:C:66:CRO:H2	2.11	0.52
1:D:15:LYS:HG2	1:D:117:LYS:HD2	1.92	0.52
1:C:66:CRO:O3	1:C:69:ASN:N	2.42	0.52
1:D:154:VAL:HG12	1:D:155:THR:N	2.25	0.52
1:A:127:LYS:HZ1	1:A:128:ASP:H	1.56	0.51
1:A:28:SER:HB2	1:A:50:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LYS:HD3	2:B:373:HOH:O	2.11	0.51
1:D:63:VAL:HG12	1:D:95:ARG:HH11	1.70	0.51
1:B:70:ARG:CZ	1:B:70:ARG:HA	2.41	0.51
1:C:171:LYS:HZ2	1:C:172:HIS:H	1.58	0.51
1:A:17:ASN:HD22	1:A:121:ASN:HD21	1.58	0.51
1:C:152:THR:HG21	2:C:267:HOH:O	2.10	0.51
1:D:98:ARG:H	1:D:98:ARG:HD3	1.74	0.51
1:B:65:PHE:CA	1:B:66:CRO:N1	2.73	0.51
1:C:167:LEU:HD12	1:C:171:LYS:HB3	1.92	0.51
1:C:36:ASN:HD22	1:C:39:GLU:H	1.57	0.51
1:A:100:GLN:NE2	1:A:174:THR:H	2.08	0.50
1:C:70:ARG:HE	1:C:73:THR:HG22	1.69	0.50
1:D:91:PHE:CZ	1:D:111:ILE:HG13	2.46	0.50
1:C:188:GLU:H	1:C:188:GLU:CD	2.14	0.50
1:A:152:THR:HG21	2:A:292:HOH:O	2.11	0.50
1:A:36:ASN:HD22	1:A:38:LEU:H	1.59	0.50
1:D:202:LYS:HG2	1:D:212:VAL:HG11	1.94	0.50
1:D:63:VAL:HG13	1:D:66:CRO:CB2	2.41	0.50
1:C:66:CRO:HD1	1:C:66:CRO:N2	2.26	0.50
1:D:171:LYS:HZ2	1:D:172:HIS:H	1.58	0.50
1:D:97:ILE:HG23	1:D:175:TYR:CD2	2.47	0.50
1:D:70:ARG:CD	1:D:73:THR:HG21	2.41	0.50
1:A:155:THR:O	1:A:155:THR:CG2	2.58	0.50
1:B:15:LYS:HZ3	1:B:117:LYS:HD2	1.77	0.50
1:D:109:SER:CB	1:D:122:VAL:HG22	2.42	0.50
1:B:180:VAL:HG11	2:B:306:HOH:O	2.12	0.50
1:B:113:LEU:HD12	1:B:117:LYS:O	2.12	0.50
1:C:11:VAL:HG23	1:C:11:VAL:O	2.11	0.50
1:D:180:VAL:HG11	2:D:288:HOH:O	2.12	0.50
1:B:18:LEU:HD22	1:B:29:MET:CE	2.41	0.49
1:D:65:PHE:C	1:D:66:CRO:HA1	2.30	0.49
1:B:85:GLN:NE2	1:B:188:GLU:OE1	2.45	0.49
1:B:36:ASN:ND2	1:B:39:GLU:H	2.10	0.49
1:B:171:LYS:HZ2	1:B:172:HIS:N	2.02	0.49
1:D:66:CRO:O3	1:D:69:ASN:N	2.46	0.49
1:D:77:GLU:HB2	1:D:78:GLU:OE2	2.12	0.49
1:A:85:GLN:NE2	1:A:188:GLU:OE1	2.43	0.49
1:A:63:VAL:CG1	1:A:95:ARG:NH1	2.76	0.49
1:C:187:VAL:HG12	2:C:296:HOH:O	2.12	0.49
1:A:171:LYS:CE	1:A:172:HIS:H	2.24	0.49
1:B:97:ILE:HD11	1:B:177:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:HG23	2:C:242:HOH:O	2.12	0.49
1:D:66:CRO:N2	1:D:66:CRO:HD1	2.28	0.48
1:B:111:ILE:N	1:B:111:ILE:HD12	2.27	0.48
1:B:200:LEU:C	1:B:200:LEU:HD23	2.34	0.48
1:A:148:GLU:HA	1:A:161[B]:CYS:HB3	1.94	0.48
1:C:36:ASN:ND2	1:C:38:LEU:H	2.11	0.48
1:D:70:ARG:CG	1:D:73:THR:HG21	2.43	0.48
1:D:87:PHE:HB3	1:D:88:PRO:HA	1.95	0.48
1:D:13:PRO:O	1:D:117:LYS:HG3	2.13	0.48
1:D:14:THR:CG2	1:D:118:PHE:HB2	2.20	0.48
1:B:141:VAL:HB	1:B:166:LYS:HG3	1.96	0.47
1:B:65:PHE:N	1:B:66:CRO:H2	2.11	0.47
1:C:14:THR:CG2	1:C:118:PHE:HB2	2.23	0.47
1:C:144:GLN:HG2	1:D:193:TYR:CE2	2.48	0.47
1:A:157:VAL:CG1	1:A:181:TYR:HB2	2.44	0.47
1:C:37:ILE:HD12	1:C:84:LEU:HD21	1.96	0.47
1:A:36:ASN:HD22	1:A:36:ASN:C	2.18	0.47
1:B:36:ASN:HD22	1:B:36:ASN:C	2.17	0.47
1:C:171:LYS:HZ3	1:C:172:HIS:H	1.62	0.47
1:D:14:THR:HG21	2:D:263:HOH:O	2.15	0.47
1:B:188:GLU:N	1:B:188:GLU:CD	2.64	0.47
1:D:70:ARG:HD2	1:D:73:THR:HG21	1.95	0.47
1:A:77:GLU:H	1:A:77:GLU:CD	2.16	0.47
1:B:65:PHE:O	1:B:66:CRO:N1	2.47	0.47
1:B:70:ARG:HH21	1:B:73:THR:HG22	1.79	0.47
1:D:203:THR:OG1	1:D:213:VAL:HG22	2.15	0.47
1:D:29:MET:HB2	1:D:65:PHE:HZ	1.79	0.47
1:D:202:LYS:HB2	1:D:202:LYS:HE3	1.70	0.47
1:B:98:ARG:HD3	1:B:98:ARG:N	2.30	0.47
1:D:70:ARG:CZ	1:D:198:HIS:HE1	2.28	0.47
1:A:50:LYS:HE2	2:A:371:HOH:O	2.15	0.46
1:D:45:LYS:HE3	2:D:285:HOH:O	2.14	0.46
1:C:197:GLN:HE22	1:D:224:THR:N	2.04	0.46
1:B:98:ARG:HB3	2:B:364:HOH:O	2.15	0.46
1:B:203:THR:O	1:B:204:ASN:HB2	2.16	0.46
1:C:154:VAL:HG12	1:C:155:THR:N	2.30	0.46
1:C:36:ASN:ND2	1:C:39:GLU:H	2.14	0.46
1:D:63:VAL:CG1	1:D:95:ARG:NH1	2.67	0.46
1:A:189:THR:O	1:A:189:THR:HG23	2.16	0.46
1:C:27:PHE:CE2	1:C:56:PHE:CZ	3.03	0.46
1:C:70:ARG:O	1:C:73:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LYS:HD2	1:D:171:LYS:HA	1.68	0.46
1:D:37:ILE:HG13	1:D:38:LEU:CD1	2.46	0.46
1:D:127:LYS:HD2	2:D:359:HOH:O	2.16	0.46
1:B:65:PHE:CA	1:B:66:CRO:H2	2.29	0.45
1:C:114:GLU:HB2	1:C:119:ILE:HG12	1.96	0.45
1:B:171:LYS:HG3	1:B:172:HIS:H	1.75	0.45
1:B:152[A]:THR:CG2	2:B:368:HOH:O	2.63	0.45
1:D:54:LEU:HG	1:D:56:PHE:CZ	2.52	0.45
1:C:98:ARG:HG3	2:C:285:HOH:O	2.16	0.45
1:D:148:GLU:HG2	1:D:150:MET:SD	2.56	0.45
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.57	0.45
1:C:97:ILE:HG23	1:C:175:TYR:CD2	2.51	0.45
1:A:15:LYS:NZ	1:A:32:VAL:HG23	2.32	0.45
1:A:65:PHE:CA	1:A:66:CRO:N1	2.78	0.45
1:C:105:ALA:O	1:C:106:ILE:HD13	2.16	0.45
1:B:54:LEU:HD12	1:B:54:LEU:H	1.81	0.45
1:B:82:TYR:CD1	1:B:187:VAL:HG11	2.50	0.45
1:B:82:TYR:HE1	1:B:187:VAL:HG11	1.75	0.45
1:B:54:LEU:HA	1:B:55:PRO:HD3	1.70	0.45
1:B:42:GLN:NE2	1:B:66:CRO:OG1	2.49	0.45
1:A:197:GLN:HE22	1:B:224:THR:N	2.12	0.44
1:B:36:ASN:HD22	1:B:38:LEU:N	2.13	0.44
1:B:144:GLN:HB3	1:B:145:PRO:HD2	2.00	0.44
1:C:20:GLY:HA2	1:C:124:PHE:O	2.17	0.44
1:C:152:THR:O	1:D:171:LYS:HE2	2.18	0.44
1:C:98:ARG:HB2	2:D:312:HOH:O	2.17	0.44
1:A:144:GLN:HB3	1:A:145:PRO:HD2	1.98	0.44
1:A:188:GLU:H	1:A:188:GLU:CD	2.20	0.44
1:B:66:CRO:HD1	1:B:66:CRO:N2	2.33	0.44
1:B:95:ARG:HB3	1:B:107:VAL:HB	1.99	0.44
1:B:9:LYS:O	1:B:12:MET:HG2	2.18	0.44
1:B:20:GLY:HA2	1:B:124:PHE:O	2.18	0.44
1:C:47:SER:HB2	1:C:211:TYR:CE1	2.52	0.44
1:A:36:ASN:ND2	1:A:39:GLU:H	2.16	0.43
1:B:36:ASN:HD21	1:B:38:LEU:HB2	1.83	0.43
1:B:87:PHE:HB3	1:B:88:PRO:HA	1.99	0.43
1:D:36:ASN:HD21	1:D:38:LEU:HB2	1.83	0.43
1:B:97:ILE:C	1:B:98:ARG:HD3	2.38	0.43
1:D:99:TYR:HA	1:D:175:TYR:HB3	1.99	0.43
1:A:65:PHE:CA	1:A:66:CRO:H2	2.32	0.43
1:C:144:GLN:HG2	1:D:193:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:GLY:HA2	1:D:127:LYS:HD2	1.99	0.43
1:D:185:LYS:HG3	1:D:186:PRO:HD2	2.00	0.43
1:A:171:LYS:HD2	1:B:153:ASN:OD1	2.19	0.43
1:D:15:LYS:NZ	1:D:117:LYS:HD2	2.33	0.43
1:B:152[A]:THR:HG22	2:B:242:HOH:O	2.17	0.43
1:B:202:LYS:HE3	1:B:202:LYS:HB2	1.87	0.43
1:B:180:VAL:HG13	2:B:326:HOH:O	2.18	0.43
1:B:13:PRO:HD2	1:B:116:GLY:O	2.18	0.43
1:B:43:GLU:HG3	1:B:43:GLU:O	2.17	0.43
1:B:48:VAL:CG2	1:B:54:LEU:HD11	2.30	0.43
1:A:23:GLY:HA2	1:A:127:LYS:CD	2.48	0.43
1:B:75:TYR:HA	1:B:76:PRO:HD3	1.94	0.43
1:A:212:VAL:HG12	1:A:213:VAL:N	2.34	0.42
1:A:22:VAL:HG23	1:A:27:PHE:HE2	1.83	0.42
1:B:152[B]:THR:HG23	1:B:191:PRO:O	2.18	0.42
1:D:16:ILE:HG12	1:D:120:VAL:HB	2.01	0.42
1:A:112:SER:HB2	2:A:338:HOH:O	2.18	0.42
1:A:63:VAL:HG12	1:A:95:ARG:NH1	2.35	0.42
1:C:158:ILE:HD13	1:C:178:ARG:NH2	2.34	0.42
1:B:82:TYR:CE2	1:B:157:VAL:HG12	2.55	0.42
1:B:130:ARG:HD2	1:B:130:ARG:HA	1.80	0.42
1:B:29:MET:HE1	1:B:65:PHE:HE1	1.85	0.42
1:B:19:GLU:OE2	1:B:28:SER:OG	2.25	0.42
1:D:152:THR:HG23	1:D:191:PRO:O	2.20	0.42
1:A:24:ASP:N	1:A:24:ASP:OD2	2.52	0.42
1:D:107:VAL:HG22	1:D:124:PHE:CD1	2.55	0.42
1:A:100:GLN:HE21	1:A:174:THR:H	1.68	0.41
1:C:153:ASN:OD1	1:D:171:LYS:HE3	2.20	0.41
1:A:93:TYR:CE1	1:A:109:SER:HB3	2.56	0.41
1:B:179:THR:HG21	1:B:181:TYR:CZ	2.55	0.41
1:B:18:LEU:C	1:B:18:LEU:HD23	2.41	0.41
1:C:75:TYR:HA	1:C:76:PRO:HD3	1.89	0.41
1:A:58:PHE:CE2	1:A:214:GLN:NE2	2.88	0.41
1:C:35:GLY:HA3	1:C:72:TYR:CE2	2.56	0.41
1:D:114:GLU:H	1:D:116:GLY:CA	2.30	0.41
1:D:127:LYS:HZ2	1:D:127:LYS:HA	1.85	0.41
1:A:170:GLY:HA3	1:C:189:THR:OG1	2.20	0.41
1:A:127:LYS:NZ	1:A:128:ASP:H	2.15	0.41
1:C:111:ILE:N	1:C:111:ILE:CD1	2.83	0.41
1:D:66:CRO:CA2	1:D:70:ARG:HH12	2.33	0.41
1:C:65:PHE:C	1:C:66:CRO:CA1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:CRO:N2	1:A:66:CRO:HD1	2.36	0.41
1:B:152[A]:THR:HG22	2:B:368:HOH:O	2.21	0.41
1:D:29:MET:CB	1:D:65:PHE:HZ	2.33	0.41
1:B:13:PRO:HB2	1:B:117:LYS:HG3	2.03	0.41
1:B:171:LYS:CE	1:B:172:HIS:H	2.33	0.41
1:B:152[B]:THR:CG2	1:B:190:MET:HB3	2.48	0.41
1:C:65:PHE:N	1:C:66:CRO:H2	2.19	0.41
1:D:106:ILE:HG12	1:D:125:LYS:HB3	2.03	0.40
1:A:179:THR:HG21	1:A:181:TYR:CZ	2.56	0.40
1:C:131:ARG:HG3	2:C:274:HOH:O	2.21	0.40
1:C:149:SER:O	1:C:159:GLY:HA2	2.22	0.40
1:D:117:LYS:HB3	1:D:117:LYS:HE2	1.92	0.40
1:B:97:ILE:HD11	1:B:177:MET:HE2	2.03	0.40
1:B:44:VAL:O	1:B:213:VAL:HA	2.21	0.40
1:D:70:ARG:CD	1:D:73:THR:CG2	2.99	0.40
1:C:107:VAL:HA	1:C:123:ASP:O	2.21	0.40
1:D:99:TYR:HA	1:D:175:TYR:CB	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	206/239 (86%)	203 (98%)	1 (0%)	2 (1%)	15	3
1	B	210/239 (88%)	205 (98%)	3 (1%)	2 (1%)	15	3
1	C	204/239 (85%)	199 (98%)	4 (2%)	1 (0%)	29	9
1	D	207/239 (87%)	201 (97%)	5 (2%)	1 (0%)	29	9
All	All	827/956 (86%)	808 (98%)	13 (2%)	6 (1%)	22	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	188	GLU
1	B	154	VAL
1	C	154	VAL
1	B	204	ASN
1	D	154	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/206 (90%)	169 (91%)	17 (9%)	9	0
1	B	188/206 (91%)	173 (92%)	15 (8%)	12	1
1	C	184/206 (89%)	173 (94%)	11 (6%)	19	2
1	D	185/206 (90%)	170 (92%)	15 (8%)	11	1
All	All	743/824 (90%)	685 (92%)	58 (8%)	13	1

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	24	ASP
1	A	36	ASN
1	A	50	LYS
1	A	54	LEU
1	A	70	ARG
1	A	73	THR
1	A	98	ARG
1	A	131	ARG
1	A	152	THR
1	A	171	LYS
1	A	187	VAL
1	A	188	GLU
1	A	190[A]	MET
1	A	190[B]	MET
1	A	202	LYS

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Mol	Chain	Res	Type
1	A	211	TYR
1	B	36	ASN
1	B	38	LEU
1	B	54	LEU
1	B	62	SER
1	B	73	THR
1	B	78[A]	GLU
1	B	78[B]	GLU
1	B	94	GLU
1	B	98	ARG
1	B	114	GLU
1	B	171	LYS
1	B	187	VAL
1	B	188	GLU
1	B	202	LYS
1	B	211	TYR
1	C	21	LEU
1	C	36	ASN
1	C	78	GLU
1	C	98	ARG
1	C	123	ASP
1	C	129	LEU
1	C	131	ARG
1	C	152	THR
1	C	188	GLU
1	C	202	LYS
1	C	211	TYR
1	D	21	LEU
1	D	54	LEU
1	D	70	ARG
1	D	84	LEU
1	D	98	ARG
1	D	127	LYS
1	D	129	LEU
1	D	144	GLN
1	D	161[A]	CYS
1	D	161[B]	CYS
1	D	188	GLU
1	D	202	LYS
1	D	211	TYR
1	D	212	VAL
1	D	213	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	100	GLN
1	A	121	ASN
1	A	138	GLN
1	A	168	GLN
1	A	197	GLN
1	A	214	GLN
1	A	215	HIS
1	B	36	ASN
1	B	42	GLN
1	B	85	GLN
1	B	100	GLN
1	B	138	GLN
1	B	168	GLN
1	B	197	GLN
1	B	215	HIS
1	C	36	ASN
1	C	96	ASN
1	C	100	GLN
1	C	138	GLN
1	C	197	GLN
1	D	36	ASN
1	D	42	GLN
1	D	85	GLN
1	D	100	GLN
1	D	168	GLN
1	D	197	GLN
1	D	214	GLN
1	D	215	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CRO	C	66	-	22,22,24	3.76	4 (18%)	27,30,34	4.03	13 (48%)
1	CRO	B	66	-	22,22,24	3.76	5 (22%)	27,30,34	3.93	14 (51%)
1	CRO	D	66	-	22,22,24	3.51	5 (22%)	27,30,34	3.73	12 (44%)
1	CRO	A	66	-	22,22,24	3.86	4 (18%)	27,30,34	3.95	12 (44%)

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
1	CRO	C	66	-	-	2/9/29/32	0/2/2/2
1	CRO	B	66	-	-	2/9/29/32	0/2/2/2
1	CRO	D	66	-	-	2/9/29/32	0/2/2/2
1	CRO	A	66	-	-	2/9/29/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	16.70	1.49	1.35
1	C	66	CRO	CB2-CA2	16.41	1.48	1.35
1	B	66	CRO	CB2-CA2	16.36	1.48	1.35
1	D	66	CRO	CB2-CA2	15.16	1.47	1.35
1	A	66	CRO	C1-N2	4.42	1.38	1.32
1	C	66	CRO	C1-N2	3.69	1.37	1.32
1	B	66	CRO	C1-N2	3.60	1.37	1.32
1	D	66	CRO	C1-N2	3.33	1.37	1.32
1	C	66	CRO	O2-C2	3.31	1.30	1.23
1	A	66	CRO	O2-C2	3.12	1.29	1.23
1	D	66	CRO	O2-C2	3.12	1.29	1.23
1	B	66	CRO	O2-C2	2.82	1.29	1.23
1	A	66	CRO	C2-N3	-2.75	1.33	1.39
1	B	66	CRO	C2-N3	-2.63	1.33	1.39
1	D	66	CRO	C2-N3	-2.56	1.33	1.39
1	B	66	CRO	CA2-C2	-2.53	1.46	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	C2-N3	-2.44	1.34	1.39
1	D	66	CRO	CA2-C2	-2.03	1.46	1.48

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-14.41	122.87	130.96
1	A	66	CRO	O2-C2-CA2	-12.91	123.71	130.96
1	B	66	CRO	O2-C2-CA2	-12.73	123.81	130.96
1	D	66	CRO	O2-C2-CA2	-11.87	124.30	130.96
1	A	66	CRO	CA2-C2-N3	11.59	108.85	103.37
1	B	66	CRO	CA2-C2-N3	10.41	108.29	103.37
1	D	66	CRO	CA2-C2-N3	9.89	108.05	103.37
1	C	66	CRO	CA2-C2-N3	9.68	107.95	103.37
1	D	66	CRO	CB2-CA2-C2	5.98	129.41	122.28
1	C	66	CRO	CB2-CA2-C2	5.16	128.44	122.28
1	D	66	CRO	CG2-CB2-CA2	-4.61	124.29	129.94
1	C	66	CRO	CA3-N3-C1	-4.56	121.69	127.16
1	B	66	CRO	CA3-N3-C1	-4.52	121.74	127.16
1	B	66	CRO	CB2-CA2-C2	4.52	127.67	122.28
1	D	66	CRO	C2-N3-C1	-4.48	105.70	107.97
1	D	66	CRO	CB2-CA2-N2	-4.14	123.09	128.83
1	A	66	CRO	CB2-CA2-C2	4.06	127.12	122.28
1	A	66	CRO	CA1-C1-N3	-4.00	119.63	124.85
1	B	66	CRO	CA1-C1-N3	-3.83	119.86	124.85
1	A	66	CRO	C2-N3-C1	-3.83	106.03	107.97
1	B	66	CRO	C2-N3-C1	-3.77	106.06	107.97
1	B	66	CRO	CA3-N3-C2	3.63	132.13	123.80
1	C	66	CRO	CA3-N3-C2	3.61	132.07	123.80
1	A	66	CRO	CA3-N3-C1	-3.53	122.93	127.16
1	C	66	CRO	C2-N3-C1	-3.47	106.21	107.97
1	C	66	CRO	CB2-CA2-N2	-3.23	124.34	128.83
1	B	66	CRO	O3-C3-CA3	-3.22	116.67	126.39
1	A	66	CRO	CA3-N3-C2	3.16	131.04	123.80
1	A	66	CRO	C2-CA2-N2	-3.07	106.78	108.93
1	C	66	CRO	O3-C3-CA3	-2.99	117.36	126.39
1	C	66	CRO	CG2-CB2-CA2	-2.98	126.29	129.94
1	A	66	CRO	O3-C3-CA3	-2.97	117.42	126.39
1	B	66	CRO	CG2-CB2-CA2	-2.90	126.39	129.94
1	B	66	CRO	C2-CA2-N2	-2.65	107.07	108.93
1	D	66	CRO	O3-C3-CA3	-2.58	118.59	126.39
1	B	66	CRO	CB2-CA2-N2	-2.57	125.25	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	C2-CA2-N2	-2.45	107.22	108.93
1	C	66	CRO	O2-C2-N3	2.43	129.18	124.35
1	C	66	CRO	CA1-C1-N3	-2.31	121.83	124.85
1	D	66	CRO	N3-C1-N2	2.26	113.02	111.45
1	A	66	CRO	CG2-CB2-CA2	-2.24	127.20	129.94
1	B	66	CRO	N3-C1-N2	2.22	112.99	111.45
1	B	66	CRO	CB1-CA1-C1	2.19	115.36	110.19
1	A	66	CRO	CB1-CA1-C1	2.10	115.15	110.19
1	C	66	CRO	CD2-CG2-CD1	2.08	120.71	117.64
1	A	66	CRO	N3-C1-N2	2.06	112.88	111.45
1	D	66	CRO	CD2-CG2-CB2	-2.05	114.24	121.22
1	D	66	CRO	C2-CA2-N2	-2.05	107.50	108.93
1	D	66	CRO	CD2-CG2-CD1	2.04	120.66	117.64
1	B	66	CRO	CD2-CG2-CD1	2.02	120.63	117.64
1	D	66	CRO	CA3-N3-C2	2.00	128.39	123.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	C3-CA3-N3-C1
1	C	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C3-CA3-N3-C1
1	B	66	CRO	C3-CA3-N3-C2
1	D	66	CRO	C3-CA3-N3-C1
1	D	66	CRO	C3-CA3-N3-C2
1	A	66	CRO	C3-CA3-N3-C1
1	A	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

4 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRO	10	0
1	B	66	CRO	11	0
1	D	66	CRO	15	0
1	A	66	CRO	10	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/239 (88%)	0.51	9 (4%) 35 39	13, 22, 39, 72	0
1	B	212/239 (88%)	0.73	11 (5%) 27 30	14, 24, 43, 65	0
1	C	211/239 (88%)	0.74	11 (5%) 27 30	20, 31, 50, 70	0
1	D	211/239 (88%)	0.87	14 (6%) 18 19	24, 35, 58, 82	0
All	All	845/956 (88%)	0.71	45 (5%) 26 29	13, 29, 51, 82	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	TYR	12.3
1	D	211	TYR	10.4
1	B	211	TYR	7.5
1	C	211	TYR	7.0
1	C	205	VAL	6.2
1	D	205	VAL	5.9
1	B	115	ASP	5.6
1	A	187	VAL	5.5
1	B	205	VAL	5.5
1	D	116	GLY	5.2
1	D	114	GLU	4.9
1	A	188	GLU	4.2
1	D	188	GLU	4.0
1	A	205	VAL	3.4
1	B	11	VAL	3.2
1	D	24	ASP	3.1
1	C	114	GLU	3.1
1	B	114	GLU	3.1
1	D	187	VAL	3.0
1	C	48	VAL	2.9
1	B	152[A]	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	131	ARG	2.8
1	A	114	GLU	2.7
1	C	180	VAL	2.6
1	D	161[A]	CYS	2.6
1	C	187	VAL	2.5
1	A	11	VAL	2.4
1	D	131	ARG	2.4
1	D	106	ILE	2.4
1	B	204	ASN	2.3
1	A	101[A]	ASP	2.2
1	D	52	ALA	2.2
1	D	9	LYS	2.2
1	C	203	THR	2.1
1	D	49	THR	2.1
1	B	203	THR	2.1
1	D	15	LYS	2.1
1	A	226	LYS	2.1
1	C	11	VAL	2.1
1	C	78	GLU	2.1
1	B	168	GLN	2.0
1	C	77	GLU	2.0
1	C	213	VAL	2.0
1	B	226	LYS	2.0
1	B	9	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRO	D	66	21/23	0.88	0.11	26,31,37,40	0
1	CRO	B	66	21/23	0.89	0.11	11,20,30,34	0
1	CRO	C	66	21/23	0.91	0.11	26,30,35,40	0
1	CRO	A	66	21/23	0.92	0.11	12,16,20,32	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.