



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:46 am BST

PDB ID : 1OL2
Title : Cyclin A binding groove inhibitor H-Arg-Arg-Leu-Asn-(p-F-Phe)-NH₂
Authors : Kontopidis, G.; Andrews, M.; McInnes, C.; Cowan, A.; Powers, H.; Innes, L.; Plater, A.; Griffiths, G.; Paterson, D.; Zheleva, D.; Lane, D.; Green, S.; Walkinshaw, M.; Fischer, P.
Deposited on : 2003-08-05
Resolution : 2.60 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

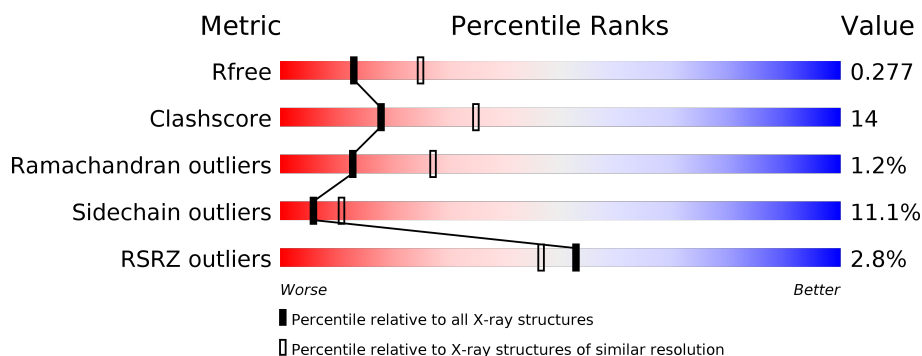
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	298	<div> <div>3%</div> <div>65% 27% 7% ..</div> </div>
1	C	298	<div> <div>4%</div> <div>68% 25% 5% ..</div> </div>
2	B	260	<div> <div>2%</div> <div>70% 24% 5% .</div> </div>
2	D	260	<div> <div>2%</div> <div>73% 22% . ..</div> </div>
3	E	6	<div> <div>33% 33% 17% 17%</div> </div>
3	F	6	<div> <div>17% 50% 33% 17%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9386 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is a protein called ARG-ARG-LEU-ASN-PFF-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	6	Total	C	F	N	O	0	0	1
			51	31	1	13	6			
3	F	6	Total	C	F	N	O	0	0	1
			51	31	1	13	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	75	Total	O	0	0
			75	75		
4	C	102	Total	O	0	0
			102	102		
4	D	85	Total	O	0	0
			85	85		

Continued on next page...

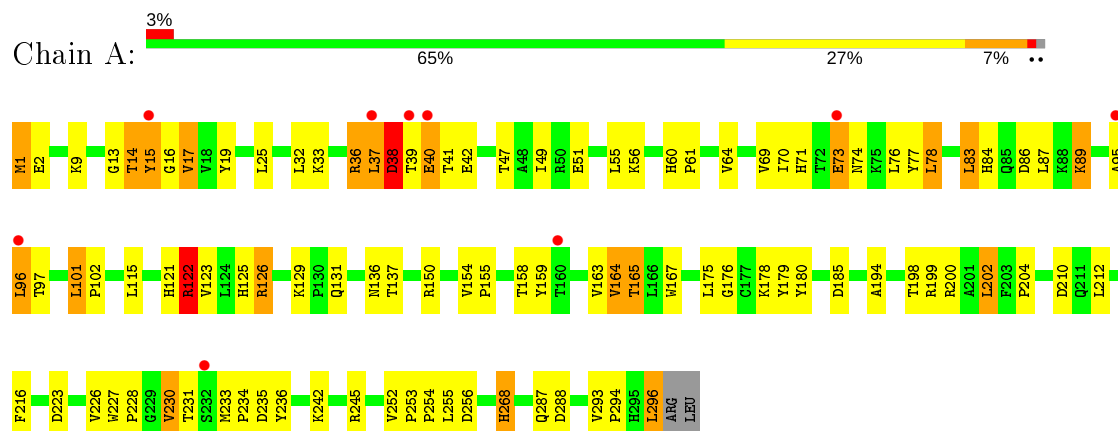
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total	O	0	0
			3	3		
4	F	3	Total	O	0	0
			3	3		

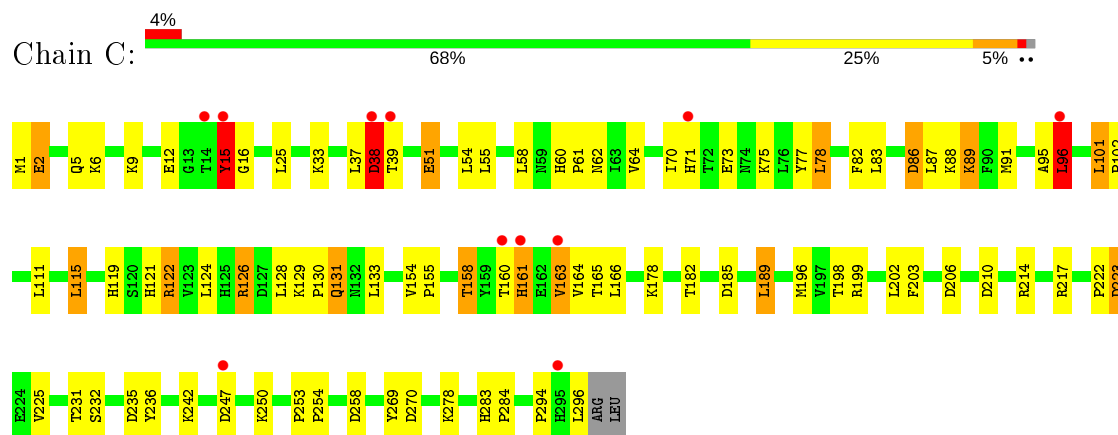
3 Residue-property plots

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 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.

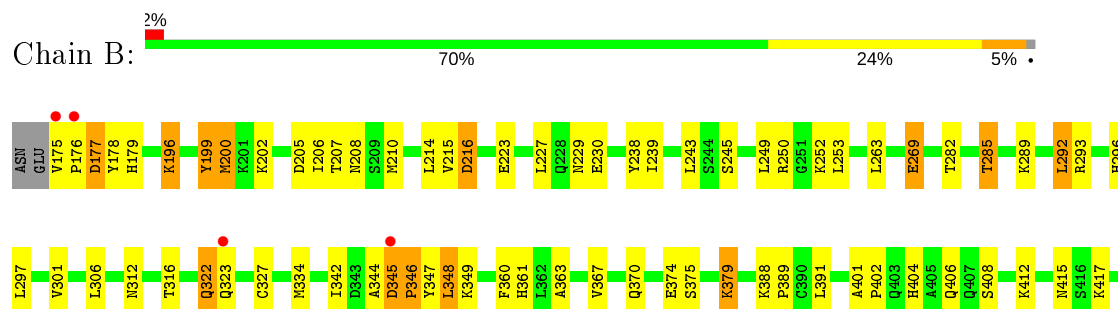
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 1: CELL DIVISION PROTEIN KINASE 2

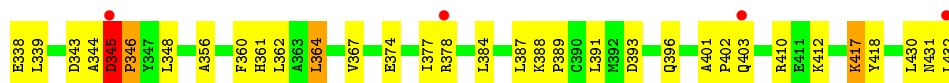
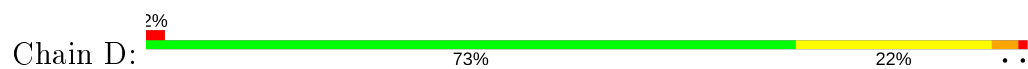


• Molecule 2: CYCLIN A2





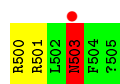
- Molecule 2: CYCLIN A2



- Molecule 3: ARG-ARG-LEU-ASN-PFF-NH2



- Molecule 3: ARG-ARG-LEU-ASN-PFF-NH2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 112.98Å 153.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 11.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (12.00-2.60) 99.6 (11.98-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.191 , 0.290 0.201 , 0.277	Depositor DCC
R_{free} test set	1220 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9386	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, PFF

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	0.59	0/2440	0.99	11/3313 (0.3%)
1	C	0.60	0/2440	0.98	8/3313 (0.2%)
2	B	0.63	0/2133	0.95	3/2897 (0.1%)
2	D	0.60	0/2134	0.99	8/2897 (0.3%)
3	E	2.03	3/37 (8.1%)	2.25	2/47 (4.3%)
3	F	2.12	3/37 (8.1%)	1.65	0/47
All	All	0.63	6/9221 (0.1%)	0.99	32/12514 (0.3%)

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	3
3	E	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	ARG	CB-CG	-7.52	1.32	1.52
3	F	501	ARG	CB-CG	-7.01	1.33	1.52
3	E	500	ARG	CB-CG	-6.92	1.33	1.52
3	E	501	ARG	CB-CG	-6.88	1.33	1.52
3	F	503	ASN	CB-CG	-6.74	1.35	1.51
3	E	503	ASN	CB-CG	-6.41	1.36	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	240	ASP	CB-CG-OD2	9.86	127.17	118.30
1	A	223	ASP	CB-CG-OD2	8.16	125.64	118.30
1	C	86	ASP	CB-CG-OD2	7.78	125.30	118.30
1	A	122	ARG	NE-CZ-NH1	-7.70	116.45	120.30
3	E	500	ARG	CA-CB-CG	7.42	129.73	113.40
2	D	343	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	235	ASP	CB-CG-OD2	7.38	124.94	118.30
2	D	345	ASP	CB-CG-OD2	7.09	124.68	118.30
1	C	258	ASP	CB-CG-OD2	7.01	124.61	118.30
2	D	393	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	150	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	256	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	288	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	1	MET	CG-SD-CE	-6.31	90.10	100.20
1	C	270	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	126	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	185	ASP	CB-CG-OD2	6.12	123.81	118.30
2	B	345	ASP	CB-CG-OD2	6.08	123.78	118.30
1	C	223	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	206	ASP	CB-CG-OD2	5.79	123.51	118.30
2	D	211	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	122	ARG	NE-CZ-NH2	5.34	122.97	120.30
2	D	181	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	216	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	205	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	243	LEU	CB-CG-CD1	-5.27	102.05	111.00
2	D	199	TYR	CB-CG-CD1	5.23	124.14	121.00
1	C	38	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	235	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	210	ASP	CB-CG-OD2	5.19	122.97	118.30
3	E	500	ARG	CB-CA-C	5.16	120.72	110.40
1	A	38	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	GLY	Peptide
1	A	163	VAL	Peptide
1	A	83	LEU	Peptide
3	E	500	ARG	Sidechain
3	E	501	ARG	Sidechain

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	2378	0	2426	93	0
1	C	2378	0	2426	73	1
2	B	2083	0	2107	47	1
2	D	2084	0	2107	41	0
3	E	51	0	49	3	0
3	F	51	0	49	3	0
4	A	93	0	0	8	0
4	B	75	0	0	6	0
4	C	102	0	0	11	0
4	D	85	0	0	6	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
All	All	9386	0	9164	246	1

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 14.

All (246) 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:37:LEU:HD13	1:A:37:LEU:O	1.10	1.23
1:A:37:LEU:CD1	1:A:37:LEU:O	1.88	1.21
1:A:15:TYR:CE2	1:A:33:LYS:HD3	1.93	1.04
1:A:15:TYR:CD2	1:A:33:LYS:HD3	1.96	1.01
3:F:503:ASN:H	3:F:503:ASN:HD22	1.01	0.97
2:B:179:HIS:NE2	2:B:379:LYS:HE2	1.84	0.93
1:A:78:LEU:HD22	4:A:2028:HOH:O	1.72	0.89
1:A:15:TYR:HD2	1:A:33:LYS:HG2	1.39	0.85
1:C:51:GLU:O	1:C:55:LEU:HB2	1.77	0.84
1:A:37:LEU:HD13	1:A:37:LEU:C	1.97	0.84
1:A:17:VAL:HB	1:A:19:TYR:CE1	2.12	0.84
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.60	0.84
1:A:73:GLU:HG3	1:C:2:GLU:HG2	1.58	0.84
2:D:387:LEU:HD22	4:D:2059:HOH:O	1.77	0.83
3:F:503:ASN:HD22	3:F:503:ASN:N	1.77	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HG23	1:C:163:VAL:O	1.80	0.80
3:F:503:ASN:ND2	3:F:503:ASN:H	1.79	0.80
3:E:500:ARG:NH2	3:E:500:ARG:HG2	1.95	0.80
2:D:345:ASP:HB2	2:D:346:PRO:HD3	1.64	0.80
1:A:95:ALA:O	1:A:96:LEU:HB2	1.83	0.76
2:D:391:LEU:HD11	4:D:2060:HOH:O	1.85	0.76
2:D:266:LYS:NZ	2:D:295:GLU:OE2	2.18	0.75
1:A:15:TYR:HD2	1:A:33:LYS:CG	2.00	0.75
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.68	0.75
1:C:15:TYR:HE2	1:C:33:LYS:HD3	1.49	0.75
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.22	0.75
1:A:15:TYR:CD2	1:A:33:LYS:CD	2.71	0.74
2:D:387:LEU:HD13	4:D:2059:HOH:O	1.88	0.73
1:A:69:VAL:HG22	4:A:2028:HOH:O	1.87	0.73
1:A:95:ALA:O	1:A:96:LEU:CB	2.37	0.72
2:B:282:THR:O	2:B:285:THR:HG22	1.88	0.72
1:A:69:VAL:HG13	4:A:2028:HOH:O	1.88	0.72
1:A:227:TRP:CD2	1:A:230:VAL:CG1	2.72	0.72
2:B:345:ASP:HB2	2:B:346:PRO:HD3	1.72	0.71
1:C:95:ALA:O	1:C:96:LEU:HB3	1.89	0.71
1:A:164:VAL:O	1:A:165:THR:CB	2.39	0.70
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.75	0.69
1:C:163:VAL:CG2	1:C:163:VAL:O	2.40	0.69
3:E:500:ARG:HG2	3:E:500:ARG:HH21	1.58	0.68
1:C:78:LEU:N	1:C:78:LEU:HD23	2.07	0.68
1:A:15:TYR:CE2	1:A:33:LYS:CD	2.76	0.67
2:B:215:VAL:HG12	2:B:342:ILE:HD13	1.76	0.67
1:A:164:VAL:O	1:A:165:THR:HB	1.95	0.67
1:A:1:MET:CE	1:A:70:ILE:HD12	2.24	0.67
1:C:15:TYR:CE2	1:C:33:LYS:HD3	2.29	0.67
1:A:227:TRP:O	1:A:230:VAL:HG22	1.94	0.67
1:C:96:LEU:HD23	4:C:2043:HOH:O	1.94	0.67
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.79	0.66
1:A:227:TRP:CG	1:A:230:VAL:HG13	2.31	0.66
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.76	0.66
2:D:182:ILE:HB	4:D:2007:HOH:O	1.96	0.66
1:A:2:GLU:HG2	1:C:73:GLU:HG3	1.77	0.66
1:A:125:HIS:O	1:A:126:ARG:HB2	1.95	0.65
1:C:198:THR:O	1:C:199:ARG:HB2	1.95	0.65
2:D:345:ASP:HB2	2:D:346:PRO:CD	2.26	0.65
2:B:297:LEU:O	2:B:301:VAL:HG23	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:HE1	1:A:47:THR:HG1	1.46	0.63
2:B:282:THR:HB	2:B:285:THR:CG2	2.27	0.63
1:A:15:TYR:CE2	1:A:51:GLU:OE1	2.51	0.63
1:C:101:LEU:CA	4:C:2044:HOH:O	2.46	0.62
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.29	0.62
2:D:315:LEU:HD23	2:D:356:ALA:HB1	1.81	0.62
1:A:15:TYR:HE2	1:A:51:GLU:OE1	1.83	0.62
2:B:196:LYS:N	2:B:196:LYS:CD	2.64	0.61
1:A:212:LEU:HD22	1:A:216:PHE:CE1	2.36	0.61
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.36	0.61
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.36	0.61
1:C:166:LEU:HB2	4:C:2073:HOH:O	2.00	0.60
2:D:193:CYS:SG	4:D:2012:HOH:O	2.56	0.60
1:A:164:VAL:O	1:A:165:THR:HG22	2.01	0.60
2:B:334:MET:HE2	4:B:2052:HOH:O	2.00	0.60
1:A:15:TYR:HD2	1:A:33:LYS:CD	2.14	0.60
1:A:137:THR:HG22	1:A:296:LEU:HD23	1.84	0.60
2:B:208:ASN:ND2	2:B:344:ALA:HB3	2.17	0.59
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.83	0.59
1:C:101:LEU:HA	4:C:2044:HOH:O	2.01	0.59
1:C:178:LYS:NZ	4:C:2064:HOH:O	2.32	0.59
1:A:15:TYR:HE2	1:A:33:LYS:HD3	1.61	0.58
1:A:175:LEU:O	1:A:234:PRO:HD2	2.03	0.58
1:A:231:THR:HA	1:A:236:TYR:CD1	2.37	0.58
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.18	0.58
1:C:91:MET:HE3	1:C:196:MET:CG	2.33	0.58
2:B:404:HIS:HD2	2:B:406:GLN:H	1.52	0.58
1:C:95:ALA:O	1:C:96:LEU:CB	2.52	0.58
2:D:401:ALA:N	2:D:402:PRO:CD	2.68	0.57
1:C:86:ASP:OD2	1:C:89:LYS:NZ	2.36	0.57
1:A:17:VAL:O	1:A:19:TYR:CD1	2.56	0.57
2:B:334:MET:CE	4:B:2052:HOH:O	2.52	0.57
1:C:91:MET:HE3	1:C:196:MET:HG2	1.86	0.57
1:A:164:VAL:O	1:A:165:THR:CG2	2.53	0.56
1:A:36:ARG:O	1:A:37:LEU:HD12	2.05	0.56
1:A:15:TYR:OH	1:A:51:GLU:OE1	2.21	0.56
1:C:231:THR:HA	1:C:236:TYR:CD1	2.41	0.56
1:A:78:LEU:HD23	1:A:78:LEU:N	2.21	0.56
1:A:14:THR:HG21	1:A:47:THR:HG21	1.87	0.56
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.88	0.56
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:CD2	4:C:2043:HOH:O	2.54	0.56
1:C:91:MET:CE	1:C:196:MET:HG2	2.37	0.55
1:A:158:THR:HA	1:A:180:TYR:CE1	2.41	0.55
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.41	0.55
2:B:346:PRO:HG2	2:B:347:TYR:CD2	2.42	0.55
1:A:121:HIS:O	1:A:123:VAL:HG23	2.07	0.54
2:D:362:LEU:HD13	4:D:2060:HOH:O	2.06	0.54
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.89	0.54
2:B:215:VAL:CG1	2:B:342:ILE:HD13	2.38	0.54
1:C:131:GLN:H	1:C:131:GLN:NE2	2.05	0.54
2:B:363:ALA:O	2:B:367:VAL:HG23	2.08	0.53
2:B:216:ASP:OD1	2:B:408:SER:HB2	2.07	0.53
1:C:91:MET:CE	1:C:196:MET:CG	2.86	0.53
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.90	0.53
1:A:15:TYR:CD2	1:A:33:LYS:HG2	2.32	0.53
1:A:64:VAL:HG23	1:A:64:VAL:O	2.08	0.53
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.72	0.53
2:B:227:LEU:HD22	2:B:269:GLU:OE2	2.09	0.52
2:B:175:VAL:HG13	2:B:177:ASP:HB2	1.91	0.52
2:B:199:TYR:CD1	2:B:199:TYR:C	2.82	0.52
2:D:338:GLU:OE1	2:D:412:LYS:NZ	2.42	0.52
1:C:1:MET:HE3	1:C:70:ILE:HD13	1.92	0.52
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.44	0.52
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.28	0.52
1:C:121:HIS:O	1:C:122:ARG:HG3	2.09	0.51
1:C:154:VAL:HG21	2:D:312:ASN:ND2	2.26	0.51
2:B:388:LYS:N	2:B:389:PRO:CD	2.74	0.51
1:A:194:ALA:CB	1:A:202:LEU:HG	2.41	0.51
1:A:14:THR:CG2	4:A:2008:HOH:O	2.59	0.51
2:B:230:GLU:OE1	2:B:312:ASN:ND2	2.30	0.51
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.91	0.51
1:A:1:MET:HE3	1:A:70:ILE:HD12	1.93	0.51
1:A:14:THR:HG21	4:A:2008:HOH:O	2.11	0.51
1:A:40:GLU:HG3	1:A:41:THR:N	2.26	0.50
1:C:164:VAL:HG23	1:C:165:THR:O	2.12	0.50
2:D:401:ALA:N	2:D:402:PRO:HD3	2.26	0.50
2:B:210:MET:HB3	3:E:504:PFF:CD2	2.41	0.50
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.41	0.50
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.45	0.50
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.26	0.50
1:C:202:LEU:HD23	1:C:203:PHE:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:C	1:C:78:LEU:HD23	2.32	0.50
1:A:227:TRP:CE3	1:A:230:VAL:HG11	2.46	0.49
2:D:430:LEU:O	2:D:431:ASN:HB2	2.10	0.49
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.93	0.49
2:B:178:TYR:O	2:B:179:HIS:C	2.50	0.49
1:C:71:HIS:HB3	2:D:296:HIS:CE1	2.47	0.49
1:A:164:VAL:CG1	1:A:165:THR:N	2.75	0.49
1:A:14:THR:OG1	4:A:2008:HOH:O	2.18	0.49
1:C:101:LEU:HD22	4:C:2044:HOH:O	2.11	0.49
2:B:252:LYS:HD2	1:C:25:LEU:O	2.12	0.49
2:B:401:ALA:N	2:B:402:PRO:CD	2.76	0.49
1:A:2:GLU:HG2	1:C:73:GLU:CG	2.43	0.49
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.48	0.48
2:B:196:LYS:N	2:B:196:LYS:HD3	2.28	0.48
1:A:198:THR:O	1:A:199:ARG:HB2	2.14	0.48
1:A:38:ASP:HB2	1:A:42:GLU:H	1.78	0.48
1:A:37:LEU:HD12	1:A:37:LEU:O	2.01	0.48
1:C:158:THR:HG21	4:C:2062:HOH:O	2.12	0.48
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.49	0.47
2:B:252:LYS:HE3	4:B:2031:HOH:O	2.13	0.47
1:C:78:LEU:N	1:C:78:LEU:CD2	2.77	0.47
1:A:137:THR:HG22	1:A:296:LEU:CD2	2.45	0.47
1:C:1:MET:CE	1:C:70:ILE:HD13	2.45	0.47
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.50	0.47
2:D:262:LEU:O	2:D:266:LYS:HG3	2.15	0.47
1:A:129:LYS:NZ	1:A:131:GLN:HE21	2.12	0.47
1:A:96:LEU:HD23	1:A:97:THR:HG23	1.97	0.47
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.97	0.47
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.46	0.46
1:A:129:LYS:HD2	1:A:131:GLN:HE21	1.80	0.46
1:A:25:LEU:HD21	2:D:293:ARG:HB3	1.96	0.46
1:C:294:PRO:HG2	1:C:296:LEU:HD21	1.97	0.46
1:A:268:HIS:ND1	4:A:2084:HOH:O	2.36	0.46
1:C:101:LEU:N	1:C:102:PRO:CD	2.79	0.46
1:C:37:LEU:O	1:C:38:ASP:C	2.53	0.46
2:B:370:GLN:HG2	4:B:2057:HOH:O	2.15	0.46
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.98	0.46
1:C:15:TYR:HB2	1:C:16:GLY:H	1.51	0.46
1:A:16:GLY:O	1:A:17:VAL:C	2.54	0.45
2:B:229:ASN:HB3	4:B:2052:HOH:O	2.14	0.45
2:D:388:LYS:HZ3	2:D:432:LEU:C	2.18	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:HG2	1:C:73:GLU:HB2	1.98	0.45
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.98	0.45
1:A:84:HIS:NE2	1:A:296:LEU:HG	2.32	0.45
1:C:131:GLN:HE21	1:C:131:GLN:H	1.65	0.45
2:B:327:CYS:HB3	4:B:2049:HOH:O	2.17	0.45
2:B:322:GLN:HG3	2:B:360:PHE:HZ	1.81	0.45
1:C:91:MET:HE3	1:C:196:MET:HG3	1.98	0.44
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.74	0.44
2:D:198:GLY:O	2:D:200:MET:N	2.50	0.44
1:C:119:HIS:CE1	1:C:182:THR:HB	2.52	0.44
1:A:101:LEU:N	1:A:102:PRO:CD	2.81	0.44
2:B:200:MET:CE	2:B:206:ILE:HD13	2.47	0.44
1:C:223:ASP:OD1	1:C:225:VAL:HB	2.18	0.43
2:D:178:TYR:O	2:D:181:ASP:HB2	2.17	0.43
2:D:329:VAL:HG22	2:D:367:VAL:HB	2.01	0.43
2:B:345:ASP:CB	2:B:346:PRO:CD	2.93	0.43
1:C:111:LEU:HD22	1:C:133:LEU:HD22	1.99	0.43
1:C:160:THR:HG22	4:C:2056:HOH:O	2.18	0.43
2:D:360:PHE:CE2	2:D:364:LEU:CD2	3.02	0.43
1:A:121:HIS:O	1:A:122:ARG:HG3	2.18	0.43
2:D:199:TYR:C	2:D:199:TYR:CD1	2.92	0.43
2:D:279:VAL:O	2:D:282:THR:OG1	2.36	0.43
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.54	0.43
1:A:129:LYS:NZ	1:A:131:GLN:NE2	2.67	0.43
1:A:194:ALA:HB1	1:A:202:LEU:HG	2.00	0.43
1:A:253:PRO:CB	1:A:254:PRO:HD3	2.48	0.43
2:B:223:GLU:OE2	2:B:412:LYS:HG3	2.17	0.43
2:D:323:GLN:O	2:D:323:GLN:HG2	2.19	0.43
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.49	0.43
1:A:15:TYR:HE2	1:A:33:LYS:CD	2.27	0.43
1:C:91:MET:HE2	1:C:196:MET:HA	2.00	0.42
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.80	0.42
2:D:315:LEU:CD2	2:D:356:ALA:HB1	2.49	0.42
1:C:160:THR:O	1:C:161:HIS:C	2.58	0.42
1:C:91:MET:CE	1:C:196:MET:HG3	2.49	0.42
2:D:401:ALA:CB	2:D:410:ARG:HD2	2.50	0.42
1:C:166:LEU:HD12	4:C:2073:HOH:O	2.20	0.42
1:C:82:PHE:C	1:C:83:LEU:HG	2.39	0.41
2:D:360:PHE:O	2:D:361:HIS:C	2.57	0.41
1:C:60:HIS:HD2	1:C:62:ASN:H	1.67	0.41
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG23	4:C:2016:HOH:O	2.21	0.41
1:A:227:TRP:O	1:A:228:PRO:C	2.58	0.41
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.79	0.41
2:B:238:TYR:N	2:B:238:TYR:CD1	2.87	0.41
1:C:253:PRO:N	1:C:254:PRO:CD	2.83	0.41
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.77	0.41
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.55	0.41
1:A:86:ASP:OD2	1:A:89:LYS:HE2	2.21	0.41
1:C:54:LEU:O	1:C:58:LEU:HG	2.20	0.41
2:D:360:PHE:O	2:D:364:LEU:HB2	2.20	0.41
1:A:122:ARG:NE	4:A:2038:HOH:O	2.52	0.41
2:B:215:VAL:HG12	2:B:342:ILE:CD1	2.49	0.41
2:B:263:LEU:HD23	2:B:263:LEU:HA	1.84	0.41
1:A:176:GLY:O	1:A:234:PRO:HG2	2.21	0.41
1:A:154:VAL:HG13	1:A:155:PRO:HD2	2.04	0.40
1:A:1:MET:HG3	1:A:77:TYR:CE1	2.56	0.40
1:A:38:ASP:HB3	1:A:41:THR:OG1	2.20	0.40
2:B:415:ASN:OD1	2:B:417:LYS:HB2	2.22	0.40
2:D:417:LYS:HG3	2:D:418:TYR:CD2	2.57	0.40
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.80	0.40
2:D:217:TRP:CH2	2:D:281:ILE:HD12	2.57	0.40
1:C:155:PRO:HD3	2:D:316:THR:HG21	2.02	0.40
2:B:322:GLN:HG3	2:B:360:PHE:CZ	2.55	0.40
1:A:73:GLU:CG	1:C:2:GLU:HG2	2.42	0.40
2:D:323:GLN:O	2:D:323:GLN:CG	2.69	0.40
2:B:239:ILE:O	2:B:243:LEU:HG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.82	0.38

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	294/298 (99%)	273 (93%)	17 (6%)	4 (1%)	11	22
1	C	294/298 (99%)	277 (94%)	14 (5%)	3 (1%)	15	32
2	B	256/260 (98%)	246 (96%)	6 (2%)	4 (2%)	9	19
2	D	256/260 (98%)	247 (96%)	7 (3%)	2 (1%)	19	39
3	E	3/6 (50%)	3 (100%)	0	0	100	100
3	F	3/6 (50%)	3 (100%)	0	0	100	100
All	All	1106/1128 (98%)	1049 (95%)	44 (4%)	13 (1%)	13	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	C	161	HIS
1	A	96	LEU
2	B	424	LEU
1	C	96	LEU
1	A	17	VAL
2	B	176	PRO
2	D	199	TYR
1	A	126	ARG
1	C	15	TYR
2	B	346	PRO
2	B	420	GLY
2	D	346	PRO

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	261/263 (99%)	227 (87%)	34 (13%)	4	7
1	C	261/263 (99%)	231 (88%)	30 (12%)	5	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	232/234 (99%)	207 (89%)	25 (11%)	6	12
2	D	232/234 (99%)	213 (92%)	19 (8%)	11	22
3	E	4/4 (100%)	3 (75%)	1 (25%)	0	1
3	F	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	994/1002 (99%)	884 (89%)	110 (11%)	6	11

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	14	THR
1	A	15	TYR
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	39	THR
1	A	40	GLU
1	A	55	LEU
1	A	56	LYS
1	A	71	HIS
1	A	73	GLU
1	A	74	ASN
1	A	76	LEU
1	A	78	LEU
1	A	87	LEU
1	A	89	LYS
1	A	101	LEU
1	A	122	ARG
1	A	159	TYR
1	A	164	VAL
1	A	200	ARG
1	A	202	LEU
1	A	226	VAL
1	A	230	VAL
1	A	233	MET
1	A	242	LYS
1	A	245	ARG
1	A	252	VAL
1	A	255	LEU
1	A	268	HIS
1	A	287	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	VAL
1	A	296	LEU
2	B	177	ASP
2	B	196	LYS
2	B	199	TYR
2	B	200	MET
2	B	202	LYS
2	B	207	THR
2	B	245	SER
2	B	249	LEU
2	B	250	ARG
2	B	269	GLU
2	B	285	THR
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	296	HIS
2	B	316	THR
2	B	322	GLN
2	B	323	GLN
2	B	348	LEU
2	B	349	LYS
2	B	374	GLU
2	B	375	SER
2	B	379	LYS
2	B	431	ASN
2	B	432	LEU
1	C	2	GLU
1	C	5	GLN
1	C	6	LYS
1	C	9	LYS
1	C	12	GLU
1	C	15	TYR
1	C	38	ASP
1	C	51	GLU
1	C	64	VAL
1	C	75	LYS
1	C	78	LEU
1	C	87	LEU
1	C	88	LYS
1	C	89	LYS
1	C	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	101	LEU
1	C	115	LEU
1	C	122	ARG
1	C	124	LEU
1	C	126	ARG
1	C	131	GLN
1	C	158	THR
1	C	163	VAL
1	C	189	LEU
1	C	217	ARG
1	C	232	SER
1	C	242	LYS
1	C	247	ASP
1	C	250	LYS
1	C	278	LYS
2	D	180	GLU
2	D	196	LYS
2	D	197	VAL
2	D	199	TYR
2	D	200	MET
2	D	201	LYS
2	D	232	LEU
2	D	281	ILE
2	D	289	LYS
2	D	292	LEU
2	D	293	ARG
2	D	323	GLN
2	D	328	LYS
2	D	345	ASP
2	D	364	LEU
2	D	378	ARG
2	D	396	GLN
2	D	403	GLN
2	D	417	LYS
3	E	500	ARG
3	F	503	ASN

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	5	GLN
1	A	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	HIS
1	A	131	GLN
2	B	208	ASN
2	B	296	HIS
2	B	404	HIS
2	B	419	HIS
2	B	431	ASN
1	C	60	HIS
1	C	131	GLN
1	C	287	GLN
2	D	208	ASN
2	D	404	HIS
2	D	431	ASN
3	F	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
3	PFF	F	504	3	11,12,13	0.76	0	12,15,17	1.16	1 (8%)
3	PFF	E	504	3	11,12,13	0.80	0	12,15,17	1.20	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PFF	F	504	3	-	2/5/6/8	0/1/1/1
3	PFF	E	504	3	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	504	PFF	CB-CA-C	-2.91	106.00	111.47
3	E	504	PFF	CE2-CZ-CE1	-2.41	119.62	122.83
3	E	504	PFF	CD1-CE1-CZ	2.22	120.66	118.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	504	PFF	N-CA-CB-CG
3	F	504	PFF	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	504	PFF	1	0

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 ⓘ

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	296/298 (99%)	-0.35	9 (3%)	50	43	21, 39, 79, 97	0
1	C	296/298 (99%)	-0.29	11 (3%)	41	34	21, 38, 86, 118	0
2	B	258/260 (99%)	-0.38	4 (1%)	72	68	25, 39, 70, 108	0
2	D	258/260 (99%)	-0.30	6 (2%)	60	54	23, 44, 71, 98	0
3	E	4/6 (66%)	-0.24	0	100	100	48, 49, 61, 79	0
3	F	4/6 (66%)	0.35	1 (25%)	0	0	38, 49, 56, 80	0
All	All	1116/1128 (98%)	-0.33	31 (2%)	53	46	21, 40, 77, 118	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	5.1
1	C	14	THR	4.1
1	C	15	TYR	3.6
1	C	163	VAL	3.6
2	B	345	ASP	3.4
1	A	73	GLU	3.2
2	D	175	VAL	3.2
2	D	323	GLN	2.9
1	A	95	ALA	2.9
1	A	37	LEU	2.9
1	A	39	THR	2.9
1	C	96	LEU	2.8
2	B	175	VAL	2.7
1	C	295	HIS	2.7
1	C	38	ASP	2.7
2	D	345	ASP	2.7
2	B	176	PRO	2.4
1	A	15	TYR	2.4
1	C	161	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	2.4
1	C	160	THR	2.3
2	D	378	ARG	2.3
1	C	71	HIS	2.2
2	D	432	LEU	2.2
3	F	503	ASN	2.2
1	A	96	LEU	2.2
1	C	247	ASP	2.1
1	A	232	SER	2.1
1	A	160	THR	2.1
2	D	403	GLN	2.1
2	B	323	GLN	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(\AA^2)	Q<0.9
3	PFF	E	504	12/13	0.86	0.18	34,47,78,87	0
3	PFF	F	504	12/13	0.90	0.15	32,48,52,54	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.