



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:41 PM UTC

PDB ID : 5OQD / pdb_00005oqd
Title : PHD2 and winged-helix domain of Polycomblike
Authors : Choi, J.; Benda, C.; Mueller, J.
Deposited on : 2017-08-11
Resolution : 2.45 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

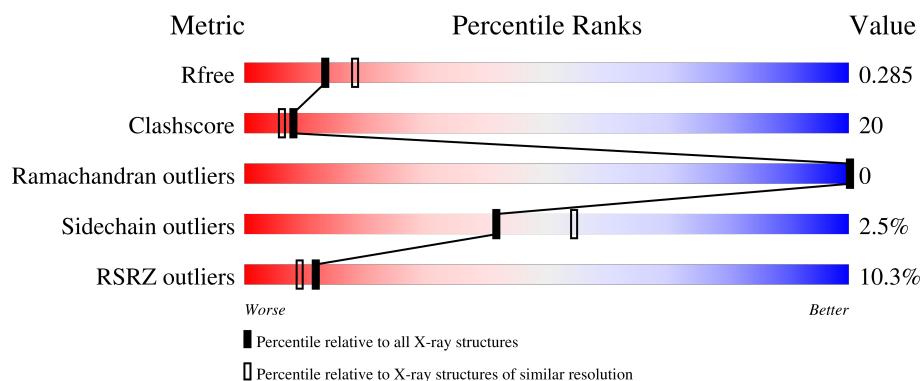
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	209	4% 66% 20% • 12%
1	B	209	6% 63% 24% • 11%
1	C	209	11% 66% 24% • 8%
1	D	209	5% 59% 27% • 11%
1	E	209	12% 61% 24% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	209	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	C	702	-	-	X	-
3	EDO	B	704	-	-	X	-
3	EDO	C	704	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9058 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 Polycomb protein Pcl.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1474	952	255	250	17			
1	A	184	Total	C	N	O	S	0	0	0
			1461	943	251	249	18			
1	C	192	Total	C	N	O	S	0	0	0
			1548	995	277	258	18			
1	D	187	Total	C	N	O	S	0	0	0
			1490	963	263	247	17			
1	E	180	Total	C	N	O	S	0	0	0
			1321	849	233	222	17			
1	F	192	Total	C	N	O	S	0	0	0
			1492	962	263	249	18			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	486	GLY	-	expression tag	UNP Q24459
B	487	PRO	-	expression tag	UNP Q24459
B	488	ASP	-	expression tag	UNP Q24459
B	489	SER	-	expression tag	UNP Q24459
B	490	MET	-	expression tag	UNP Q24459
A	486	GLY	-	expression tag	UNP Q24459
A	487	PRO	-	expression tag	UNP Q24459
A	488	ASP	-	expression tag	UNP Q24459
A	489	SER	-	expression tag	UNP Q24459
A	490	MET	-	expression tag	UNP Q24459
C	486	GLY	-	expression tag	UNP Q24459
C	487	PRO	-	expression tag	UNP Q24459
C	488	ASP	-	expression tag	UNP Q24459
C	489	SER	-	expression tag	UNP Q24459
C	490	MET	-	expression tag	UNP Q24459
D	486	GLY	-	expression tag	UNP Q24459
D	487	PRO	-	expression tag	UNP Q24459

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	488	ASP	-	expression tag	UNP Q24459
D	489	SER	-	expression tag	UNP Q24459
D	490	MET	-	expression tag	UNP Q24459
E	486	GLY	-	expression tag	UNP Q24459
E	487	PRO	-	expression tag	UNP Q24459
E	488	ASP	-	expression tag	UNP Q24459
E	489	SER	-	expression tag	UNP Q24459
E	490	MET	-	expression tag	UNP Q24459
F	486	GLY	-	expression tag	UNP Q24459
F	487	PRO	-	expression tag	UNP Q24459
F	488	ASP	-	expression tag	UNP Q24459
F	489	SER	-	expression tag	UNP Q24459
F	490	MET	-	expression tag	UNP Q24459

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

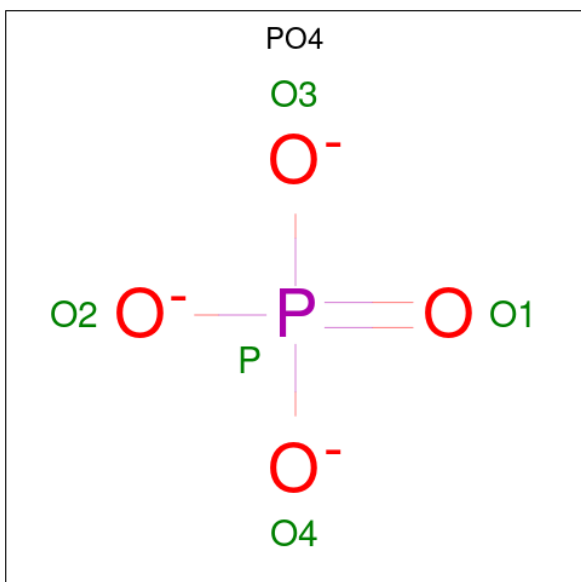
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total 2 Zn 2	0	0
2	A	2	Total 2 Zn 2	0	0
2	C	2	Total 2 Zn 2	0	0
2	D	2	Total 2 Zn 2	0	0
2	E	2	Total 2 Zn 2	0	0
2	F	2	Total 2 Zn 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

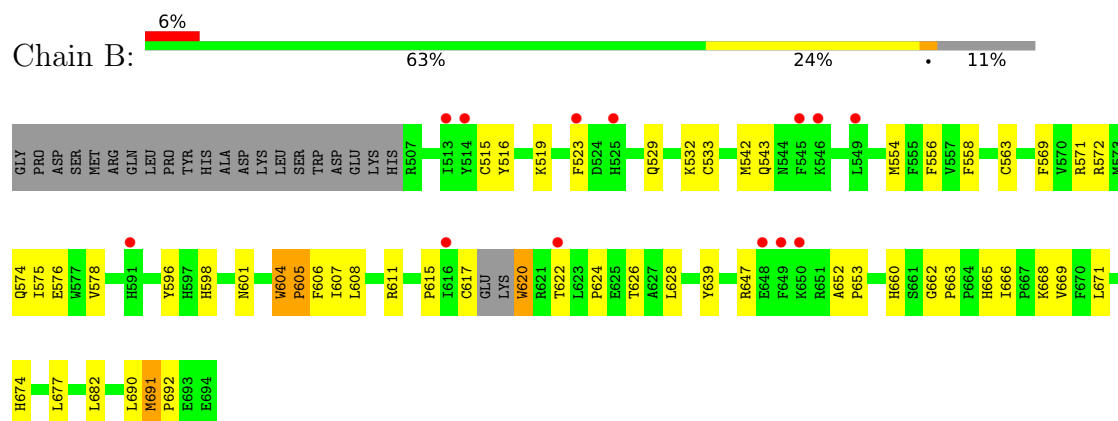
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	45	Total	O	0	0
			45	45		
5	A	52	Total	O	0	0
			52	52		
5	C	47	Total	O	0	0
			47	47		
5	D	42	Total	O	0	0
			42	42		
5	E	9	Total	O	0	0
			9	9		
5	F	35	Total	O	0	0
			35	35		

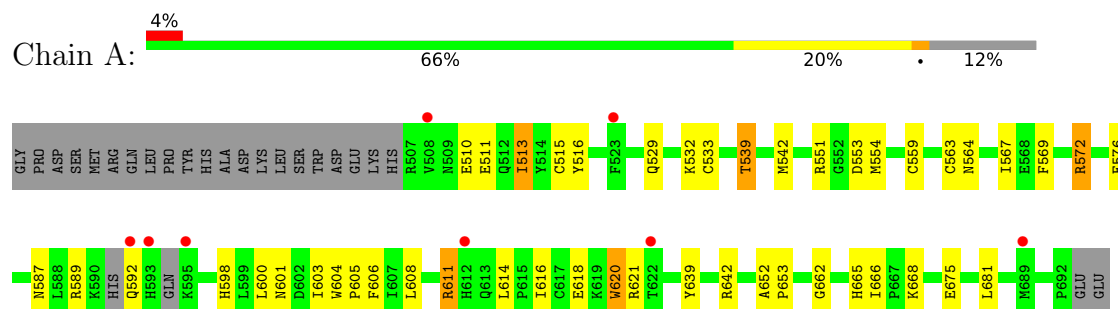
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

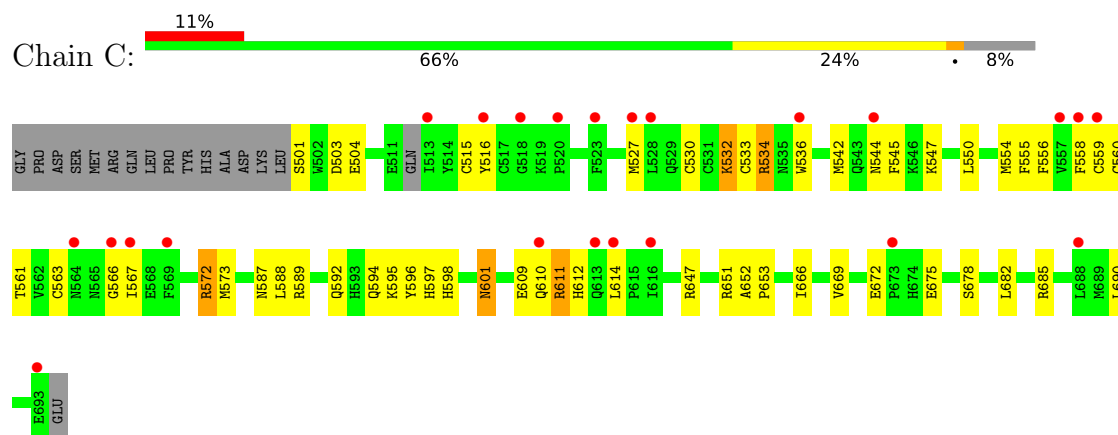
• Molecule 1: Polycomb protein Pcl



• Molecule 1: Polycomb protein Pcl

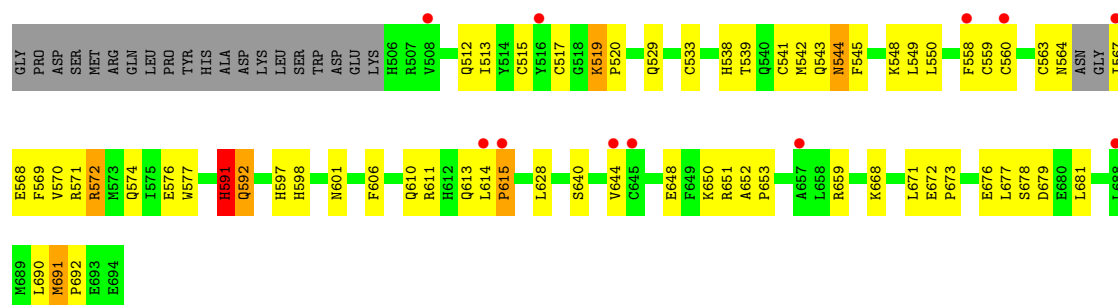


• Molecule 1: Polycomb protein Pcl



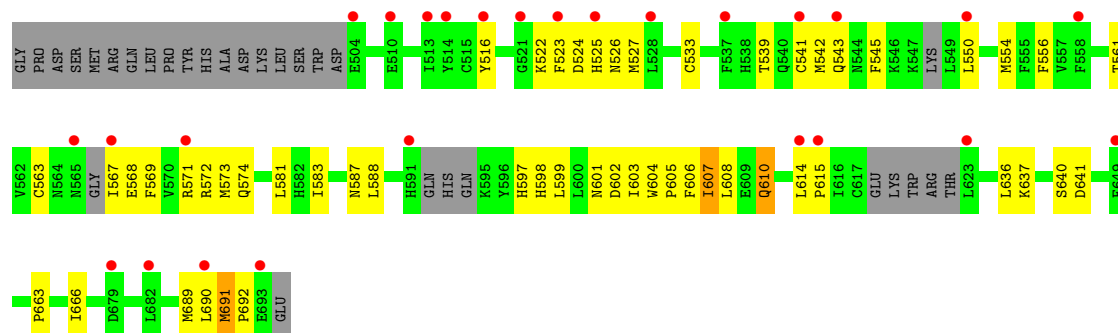
- Molecule 1: Polycomb protein Pcl

Chain D: 



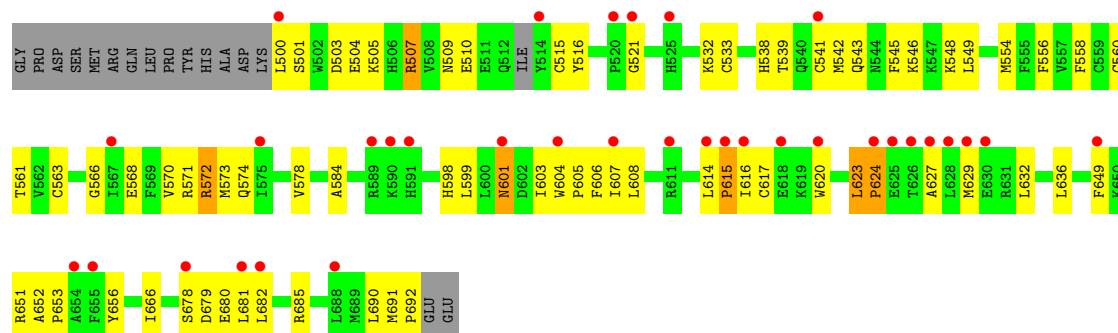
- Molecule 1: Polycomb protein Pcl

Chain E: 



- Molecule 1: Polycomb protein Pcl

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	307.42Å 53.12Å 86.84Å 90.00° 105.47° 90.00°	Depositor
Resolution (Å)	83.69 – 2.45 83.69 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.5 (83.69-2.45) 95.2 (83.69-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.236 , 0.278 0.249 , 0.285	Depositor DCC
R_{free} test set	2493 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9058	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% 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: PO4, ZN, EDO

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	0.52	2/1502 (0.1%)	0.81	6/2039 (0.3%)
1	B	0.58	4/1516 (0.3%)	0.89	9/2060 (0.4%)
1	C	0.47	2/1595 (0.1%)	0.84	7/2160 (0.3%)
1	D	0.60	8/1534 (0.5%)	1.00	15/2083 (0.7%)
1	E	0.49	4/1356 (0.3%)	0.84	4/1847 (0.2%)
1	F	0.58	6/1538 (0.4%)	1.00	10/2094 (0.5%)
All	All	0.54	26/9041 (0.3%)	0.90	51/12283 (0.4%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	615	PRO	N-CD	6.75	1.57	1.47
1	B	691	MET	C-N	6.33	1.41	1.33
1	F	614	LEU	C-N	6.27	1.40	1.33
1	E	614	LEU	C-N	6.26	1.40	1.33
1	A	652	ALA	C-N	6.25	1.41	1.33
1	D	519	LYS	C-N	5.76	1.41	1.33
1	E	691	MET	C-N	5.72	1.41	1.33
1	F	623	LEU	C-N	5.66	1.41	1.33
1	E	615	PRO	N-CD	5.51	1.55	1.47
1	F	652	ALA	C-N	5.50	1.40	1.33
1	D	652	ALA	C-N	5.49	1.40	1.33
1	C	652	ALA	C-N	5.48	1.40	1.33
1	B	624	PRO	N-CD	5.47	1.55	1.47
1	D	691	MET	C-N	5.46	1.41	1.33
1	D	672	GLU	C-N	5.38	1.40	1.33
1	F	624	PRO	N-CD	5.38	1.55	1.47
1	E	692	PRO	N-CD	5.36	1.55	1.47
1	F	615	PRO	N-CD	5.36	1.55	1.47
1	F	653	PRO	N-CD	5.34	1.55	1.47
1	B	692	PRO	N-CD	5.34	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	653	PRO	N-CD	5.29	1.55	1.47
1	C	653	PRO	N-CD	5.21	1.55	1.47
1	D	673	PRO	N-CD	5.16	1.54	1.47
1	A	653	PRO	N-CD	5.16	1.54	1.47
1	D	692	PRO	N-CD	5.15	1.54	1.47
1	B	605	PRO	N-CD	5.13	1.54	1.47

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	LYS	N-CA-C	10.20	122.16	111.14
1	F	532	LYS	N-CA-C	9.57	121.47	111.14
1	A	532	LYS	N-CA-C	9.40	121.29	111.14
1	C	532	LYS	N-CA-C	8.06	120.15	111.36
1	F	601	ASN	N-CA-C	7.84	119.91	111.36
1	B	691	MET	CA-C-N	-7.39	113.07	120.31
1	B	691	MET	C-N-CA	-7.39	113.07	120.31
1	C	601	ASN	N-CA-C	7.20	119.21	111.36
1	F	548	LYS	N-CA-C	-7.10	98.12	109.76
1	E	614	LEU	CA-C-N	-7.08	113.37	120.31
1	E	614	LEU	C-N-CA	-7.08	113.37	120.31
1	B	622	THR	N-CA-C	7.05	118.96	111.28
1	F	614	LEU	CA-C-N	-6.86	113.59	120.31
1	F	614	LEU	C-N-CA	-6.86	113.59	120.31
1	E	691	MET	CA-C-N	-6.60	113.18	119.85
1	E	691	MET	C-N-CA	-6.60	113.18	119.85
1	A	652	ALA	CA-C-N	-6.58	112.99	119.90
1	A	652	ALA	C-N-CA	-6.58	112.99	119.90
1	D	691	MET	CA-C-N	-6.49	113.10	119.78
1	D	691	MET	C-N-CA	-6.49	113.10	119.78
1	D	519	LYS	CA-C-N	-6.46	113.32	119.85
1	D	519	LYS	C-N-CA	-6.46	113.32	119.85
1	D	615	PRO	CA-N-CD	-6.46	102.96	112.00
1	F	652	ALA	CA-C-N	-6.42	113.34	119.76
1	F	652	ALA	C-N-CA	-6.42	113.34	119.76
1	F	623	LEU	CA-C-N	-6.32	113.46	119.85
1	F	623	LEU	C-N-CA	-6.32	113.46	119.85
1	C	652	ALA	CA-C-N	-6.30	113.46	119.76
1	C	652	ALA	C-N-CA	-6.30	113.46	119.76
1	D	652	ALA	CA-C-N	-6.28	113.48	119.76
1	D	652	ALA	C-N-CA	-6.28	113.48	119.76
1	D	591	HIS	N-CA-C	6.23	117.87	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	652	ALA	N-CA-C	-6.14	101.61	110.08
1	D	544	ASN	N-CA-C	6.09	120.58	112.30
1	A	662	GLY	CA-C-N	5.93	126.49	120.38
1	A	662	GLY	C-N-CA	5.93	126.49	120.38
1	D	592	GLN	N-CA-C	5.68	117.55	111.36
1	F	504	GLU	N-CA-C	5.63	117.50	111.36
1	C	504	GLU	N-CA-C	5.47	117.33	111.36
1	D	651	ARG	N-CA-C	-5.44	101.98	110.42
1	C	544	ASN	N-CA-C	5.42	117.18	111.28
1	B	604	TRP	CA-C-N	-5.36	113.10	119.05
1	B	604	TRP	C-N-CA	-5.36	113.10	119.05
1	D	672	GLU	CA-C-N	-5.34	113.40	119.28
1	D	672	GLU	C-N-CA	-5.34	113.40	119.28
1	D	614	LEU	CA-C-N	-5.12	113.45	119.84
1	D	614	LEU	C-N-CA	-5.12	113.45	119.84
1	C	587	ASN	N-CA-C	5.09	116.91	111.36
1	A	603	ILE	N-CA-C	-5.08	106.73	111.45
1	B	662	GLY	CA-C-N	5.04	125.57	120.38
1	B	662	GLY	C-N-CA	5.04	125.57	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1461	0	1335	41	0
1	B	1474	0	1357	50	0
1	C	1548	0	1416	52	1
1	D	1490	0	1367	74	0
1	E	1321	0	1117	52	0
1	F	1492	0	1318	72	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	2	0
2	D	2	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	B	8	0	12	6	0
3	C	8	0	12	6	0
3	F	4	0	6	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	52	0	0	5	0
5	B	45	0	0	2	0
5	C	47	0	0	4	3
5	D	42	0	0	5	1
5	E	9	0	0	2	0
5	F	35	0	0	9	3
All	All	9058	0	7940	327	5

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 20.

All (327) 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:D:538:HIS:O	1:D:542:MET:HG3	1.39	1.23
1:C:611:ARG:HG3	3:C:704:EDO:H12	1.23	1.17
1:F:543:GLN:HE22	1:F:561:THR:CG2	1.59	1.14
1:B:617:CYS:C	1:B:620:TRP:N	2.07	1.11
1:F:543:GLN:NE2	1:F:561:THR:CG2	2.19	1.06
1:F:615:PRO:HB2	1:F:691:MET:HE3	1.35	1.06
1:F:604:TRP:CZ2	1:F:608:LEU:HD11	1.90	1.04
1:A:589:ARG:O	1:A:592:GLN:N	1.92	1.02
1:C:612:HIS:HB3	3:C:704:EDO:H11	1.41	1.01
1:E:598:HIS:HD2	1:E:601:ASN:H	1.01	0.97
1:C:563:CYS:HG	2:C:702:ZN:ZN	0.73	0.96
1:B:523:PHE:CD2	1:B:554:MET:HE1	2.01	0.96
1:F:543:GLN:NE2	1:F:561:THR:HG21	1.80	0.95
1:C:675:GLU:OE2	1:C:685:ARG:NH1	1.99	0.94
1:F:554:MET:HB2	1:F:666:ILE:HD13	1.53	0.91
1:D:567:ILE:HD11	1:E:606:PHE:CD1	2.06	0.91
1:A:642:ARG:HD3	1:A:665:HIS:CE1	2.07	0.90
1:E:598:HIS:CD2	1:E:601:ASN:H	1.90	0.89
1:C:611:ARG:CG	3:C:704:EDO:H12	2.01	0.89
1:D:533:CYS:HB3	1:D:563:CYS:SG	2.12	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:CYS:HB3	1:E:563:CYS:SG	2.14	0.88
1:C:561:THR:O	1:C:566:GLY:N	2.08	0.86
1:E:637:LYS:O	1:E:640:SER:OG	1.93	0.86
1:A:533:CYS:HB3	1:A:563:CYS:SG	2.17	0.83
1:F:616:ILE:HG13	5:F:807:HOH:O	1.77	0.83
1:D:592:GLN:OE1	1:D:597:HIS:ND1	2.12	0.82
1:E:598:HIS:HB3	1:E:601:ASN:HB2	1.60	0.81
1:D:538:HIS:O	1:D:542:MET:CG	2.26	0.81
1:F:561:THR:HB	1:F:566:GLY:HA2	1.61	0.81
1:B:543:GLN:OE1	1:C:609:GLU:HG2	1.81	0.81
1:B:523:PHE:HD2	1:B:554:MET:HE1	1.46	0.80
1:F:538:HIS:O	1:F:542:MET:HG3	1.82	0.80
1:D:567:ILE:HD11	1:E:606:PHE:CE1	2.18	0.79
1:D:545:PHE:HE2	1:D:549:LEU:HD11	1.49	0.78
1:E:603:ILE:O	1:E:607:ILE:HG13	1.82	0.78
1:B:554:MET:HB2	1:B:666:ILE:HD12	1.65	0.78
1:E:573:MET:HA	1:E:690:LEU:HD23	1.65	0.78
1:E:561:THR:HG23	1:E:567:ILE:N	2.00	0.77
1:C:563:CYS:SG	2:C:702:ZN:ZN	1.73	0.75
1:D:542:MET:HE3	1:D:558:PHE:CZ	2.22	0.75
1:F:554:MET:HB2	1:F:666:ILE:CD1	2.16	0.75
1:D:542:MET:HE3	1:D:558:PHE:CE1	2.22	0.75
1:B:671:LEU:HD12	1:B:677:LEU:CD2	2.16	0.75
1:D:678:SER:CB	1:D:681:LEU:HG	2.17	0.74
1:B:671:LEU:HD12	1:B:677:LEU:HD21	1.68	0.74
1:F:533:CYS:HB3	1:F:563:CYS:SG	2.28	0.74
1:C:533:CYS:N	1:C:563:CYS:SG	2.60	0.74
1:E:598:HIS:HD2	1:E:601:ASN:N	1.83	0.73
1:F:649:PHE:HD2	1:F:651:ARG:NH2	1.87	0.73
1:C:532:LYS:CB	1:C:563:CYS:SG	2.76	0.73
1:B:529:GLN:O	3:B:704:EDO:C1	2.37	0.73
1:A:614:LEU:O	1:A:621:ARG:NH2	2.21	0.73
1:C:612:HIS:HB3	3:C:704:EDO:C1	2.19	0.72
1:F:542:MET:HE3	1:F:558:PHE:CE1	2.24	0.72
1:F:543:GLN:HE22	1:F:561:THR:HG22	1.53	0.72
1:F:685:ARG:NH2	5:F:802:HOH:O	2.24	0.71
1:F:556:PHE:CE2	1:F:572:ARG:HG2	2.26	0.71
1:D:570:VAL:CG2	5:D:841:HOH:O	2.39	0.71
1:B:671:LEU:CD1	1:B:677:LEU:CD2	2.68	0.70
1:F:604:TRP:CZ2	1:F:608:LEU:CD1	2.71	0.70
1:C:592:GLN:NE2	5:C:801:HOH:O	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:617:CYS:HB3	1:F:620:TRP:HD1	1.57	0.70
1:D:678:SER:H	1:D:681:LEU:HD12	1.57	0.69
1:F:629:MET:CE	1:F:632:LEU:HD12	2.21	0.69
1:F:624:PRO:HG2	1:F:627:ALA:HB2	1.74	0.69
1:D:512:GLN:HG2	1:D:520:PRO:CG	2.21	0.69
1:C:682:LEU:HD12	1:C:690:LEU:HD11	1.75	0.69
1:D:570:VAL:HG21	5:D:841:HOH:O	1.92	0.69
1:C:561:THR:HB	1:C:566:GLY:HA2	1.73	0.68
1:D:615:PRO:HD2	1:D:615:PRO:O	1.93	0.68
1:D:550:LEU:HD11	1:D:610:GLN:HG2	1.75	0.68
1:A:589:ARG:C	1:A:592:GLN:N	2.51	0.68
1:D:545:PHE:CE2	1:D:549:LEU:HD11	2.29	0.68
1:D:512:GLN:HG2	1:D:520:PRO:HG3	1.76	0.67
1:B:665:HIS:CG	1:A:665:HIS:HD2	2.12	0.67
1:D:574:GLN:HB2	1:D:691:MET:HE2	1.77	0.67
1:F:543:GLN:NE2	1:F:561:THR:HG23	2.10	0.67
1:F:601:ASN:O	1:F:605:PRO:HG2	1.94	0.67
1:C:545:PHE:HE1	1:C:547:LYS:O	1.77	0.67
1:A:620:TRP:HE3	1:A:620:TRP:HA	1.60	0.66
1:D:517:CYS:SG	1:D:519:LYS:HB2	2.34	0.66
1:D:574:GLN:HA	1:D:691:MET:HE3	1.76	0.66
1:D:563:CYS:SG	2:D:702:ZN:ZN	1.85	0.66
1:E:599:LEU:HD12	1:E:603:ILE:HB	1.77	0.65
1:A:620:TRP:HA	1:A:620:TRP:CE3	2.30	0.65
1:B:575:ILE:HG12	1:B:615:PRO:O	1.96	0.65
1:B:529:GLN:OE1	1:B:668:LYS:NZ	2.30	0.65
1:F:571:ARG:NH1	1:F:691:MET:O	2.30	0.65
1:C:501:SER:OG	1:C:503:ASP:OD1	2.15	0.65
1:D:539:THR:HG23	1:D:545:PHE:HB3	1.79	0.65
1:F:624:PRO:HG2	1:F:627:ALA:CB	2.27	0.64
1:E:604:TRP:NE1	1:E:608:LEU:HD11	2.13	0.64
1:E:641:ASP:N	1:E:641:ASP:OD1	2.30	0.64
1:D:549:LEU:N	1:D:549:LEU:HD12	2.12	0.64
1:A:618:GLU:HG2	5:A:851:HOH:O	1.98	0.63
1:F:629:MET:HE1	1:F:632:LEU:HD12	1.80	0.63
1:A:604:TRP:HB3	1:A:605:PRO:HD3	1.79	0.63
1:C:669:VAL:H	3:C:705:EDO:H22	1.64	0.63
1:C:647:ARG:HA	5:C:811:HOH:O	1.99	0.63
1:D:515:CYS:C	1:D:517:CYS:H	2.07	0.63
1:F:649:PHE:CD2	1:F:651:ARG:NH2	2.65	0.62
1:A:642:ARG:HD3	1:A:665:HIS:HE1	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:CYS:HB3	1:C:563:CYS:SG	2.39	0.61
1:C:554:MET:HB2	1:C:666:ILE:CD1	2.29	0.61
1:D:611:ARG:NH2	5:D:804:HOH:O	2.32	0.61
1:B:574:GLN:HG3	1:B:691:MET:HG3	1.81	0.61
1:E:542:MET:HE2	1:E:545:PHE:HD2	1.66	0.61
1:D:574:GLN:HA	1:D:691:MET:CE	2.30	0.61
1:D:648:GLU:HG2	1:D:648:GLU:O	2.00	0.61
1:D:671:LEU:HD12	1:D:677:LEU:HD23	1.83	0.61
1:C:545:PHE:CE1	1:C:547:LYS:O	2.53	0.60
1:E:526:ASN:O	1:E:539:THR:HG23	2.01	0.60
1:D:571:ARG:NH1	1:D:691:MET:O	2.35	0.60
1:D:529:GLN:OE1	1:D:668:LYS:NZ	2.30	0.60
1:D:615:PRO:O	1:D:615:PRO:CD	2.49	0.60
1:B:529:GLN:O	3:B:704:EDO:H12	2.02	0.59
1:C:647:ARG:NH2	1:C:651:ARG:O	2.35	0.59
1:C:592:GLN:HE21	1:C:597:HIS:CD2	2.20	0.58
1:E:556:PHE:CE1	1:E:572:ARG:HD2	2.37	0.58
1:A:616:ILE:HG12	1:A:621:ARG:HH21	1.68	0.58
1:F:598:HIS:HD2	1:F:601:ASN:CG	2.11	0.58
1:B:529:GLN:O	3:B:704:EDO:H11	2.04	0.57
1:A:529:GLN:OE1	1:A:668:LYS:NZ	2.34	0.57
1:D:559:CYS:HB3	1:D:569:PHE:HB3	1.86	0.57
1:C:561:THR:HA	1:C:567:ILE:O	2.04	0.57
1:D:543:GLN:N	1:D:568:GLU:OE2	2.38	0.57
1:D:606:PHE:O	1:D:610:GLN:NE2	2.37	0.57
1:C:530:CYS:SG	1:C:559:CYS:HA	2.45	0.57
1:C:542:MET:SD	1:C:545:PHE:HB2	2.44	0.57
1:B:639:TYR:CE2	1:A:668:LYS:HG3	2.40	0.56
1:F:509:ASN:O	5:F:801:HOH:O	2.18	0.56
1:B:543:GLN:CD	1:C:609:GLU:HG2	2.30	0.56
1:B:682:LEU:HD12	1:B:690:LEU:HD21	1.87	0.56
1:B:668:LYS:HG3	1:A:639:TYR:CE2	2.41	0.56
1:C:589:ARG:O	1:C:592:GLN:O	2.24	0.56
1:F:629:MET:HE2	1:F:632:LEU:HD12	1.86	0.56
1:C:555:PHE:HB2	1:C:572:ARG:HH21	1.69	0.56
1:D:574:GLN:CB	1:D:691:MET:HE2	2.36	0.56
1:E:604:TRP:N	1:E:605:PRO:HD2	2.20	0.55
1:C:647:ARG:HH21	1:C:651:ARG:C	2.13	0.55
1:D:539:THR:O	1:D:542:MET:HB2	2.07	0.55
1:F:598:HIS:HB3	1:F:601:ASN:HB2	1.89	0.55
1:F:616:ILE:HG22	1:F:617:CYS:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:SER:O	1:C:682:LEU:HG	2.07	0.55
1:C:592:GLN:NE2	1:C:597:HIS:CD2	2.74	0.55
1:D:576:GLU:OE2	1:D:576:GLU:HA	2.06	0.55
1:F:545:PHE:HE1	1:F:570:VAL:HG11	1.72	0.54
1:D:559:CYS:SG	1:D:564:ASN:HB3	2.48	0.54
1:B:653:PRO:HG3	1:A:511:GLU:OE1	2.07	0.54
1:B:620:TRP:N	1:B:620:TRP:CD1	2.75	0.54
1:F:598:HIS:CD2	1:F:601:ASN:CG	2.86	0.54
1:D:515:CYS:C	1:D:517:CYS:N	2.64	0.54
5:D:804:HOH:O	1:F:649:PHE:HE2	1.90	0.54
1:D:678:SER:CB	1:D:681:LEU:CD1	2.86	0.54
1:E:571:ARG:NH1	1:E:691:MET:O	2.40	0.54
1:D:572:ARG:HG2	1:D:691:MET:HG3	1.90	0.54
1:F:574:GLN:HA	1:F:691:MET:HE2	1.90	0.54
1:B:604:TRP:CD1	1:B:608:LEU:HD23	2.42	0.53
1:F:507:ARG:NH1	5:F:805:HOH:O	2.41	0.53
1:F:678:SER:HB2	1:F:681:LEU:HD23	1.90	0.53
1:B:533:CYS:HB3	1:B:563:CYS:SG	2.48	0.53
1:B:669:VAL:O	3:B:704:EDO:C2	2.57	0.53
1:F:572:ARG:HD2	1:F:615:PRO:HG3	1.89	0.53
1:F:560:CYS:HA	3:F:703:EDO:H21	1.89	0.53
1:B:574:GLN:CG	1:B:691:MET:HG3	2.38	0.53
1:A:606:PHE:C	1:A:606:PHE:CD2	2.86	0.53
1:D:571:ARG:HG2	1:D:690:LEU:HD13	1.90	0.53
1:F:538:HIS:HB2	1:F:541:CYS:SG	2.48	0.53
1:F:598:HIS:CD2	1:F:601:ASN:HB2	2.43	0.53
1:E:604:TRP:NE1	1:E:608:LEU:CD1	2.72	0.53
1:D:515:CYS:HB3	1:D:517:CYS:SG	2.49	0.52
1:D:560:CYS:O	1:D:564:ASN:O	2.27	0.52
1:E:524:ASP:OD1	1:E:525:HIS:N	2.42	0.52
1:B:665:HIS:CG	1:A:665:HIS:CD2	2.96	0.52
1:D:610:GLN:HB3	1:D:613:GLN:HB2	1.92	0.52
1:F:507:ARG:HD2	1:F:507:ARG:N	2.25	0.52
1:D:678:SER:CB	1:D:681:LEU:CG	2.85	0.52
1:B:665:HIS:CD2	1:A:665:HIS:CD2	2.99	0.51
1:D:513:ILE:O	1:D:520:PRO:HA	2.11	0.51
1:A:604:TRP:CE2	1:A:608:LEU:HD11	2.46	0.51
1:E:574:GLN:HB3	1:E:689:MET:O	2.11	0.51
1:F:539:THR:CG2	1:F:545:PHE:CD2	2.94	0.51
1:B:669:VAL:O	3:B:704:EDO:H22	2.10	0.51
1:E:516:TYR:CE2	1:E:541:CYS:HB3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:PHE:CE2	1:B:572:ARG:HD3	2.46	0.50
1:F:573:MET:HA	1:F:690:LEU:HD23	1.93	0.50
1:D:644:VAL:HG22	1:D:659:ARG:HG2	1.93	0.50
1:E:604:TRP:CE2	1:E:608:LEU:HD11	2.47	0.50
1:F:571:ARG:NH2	1:F:679:ASP:OD2	2.44	0.50
1:D:538:HIS:HB2	1:D:541:CYS:SG	2.51	0.50
1:D:539:THR:HG23	1:D:545:PHE:HD2	1.77	0.50
1:F:572:ARG:NH1	1:F:615:PRO:HD3	2.26	0.50
1:C:561:THR:HB	1:C:566:GLY:CA	2.42	0.50
1:E:522:LYS:O	1:E:527:MET:HG3	2.12	0.50
1:F:538:HIS:HB2	1:F:541:CYS:HB2	1.94	0.49
1:B:598:HIS:HB3	1:B:601:ASN:HB2	1.93	0.49
1:B:604:TRP:CH2	1:B:628:LEU:HD23	2.48	0.49
1:D:678:SER:CB	1:D:681:LEU:HD12	2.42	0.49
1:F:510:GLU:HB3	5:F:809:HOH:O	2.12	0.49
1:A:642:ARG:NH1	1:A:665:HIS:ND1	2.61	0.49
1:D:560:CYS:SG	1:D:563:CYS:SG	3.11	0.49
1:B:606:PHE:CD1	1:B:606:PHE:C	2.91	0.49
1:D:592:GLN:HB2	1:D:597:HIS:HE1	1.76	0.49
1:B:596:TYR:OH	1:A:510:GLU:HG2	2.13	0.48
1:C:515:CYS:SG	1:C:516:TYR:N	2.86	0.48
1:C:669:VAL:O	3:C:705:EDO:H12	2.13	0.48
1:A:553:ASP:OD1	1:A:572:ARG:NH2	2.45	0.48
1:B:523:PHE:CD2	1:B:554:MET:CE	2.87	0.48
1:B:607:ILE:O	1:B:611:ARG:N	2.46	0.48
1:A:551:ARG:O	1:A:587:ASN:ND2	2.45	0.48
1:E:569:PHE:HA	5:E:804:HOH:O	2.14	0.48
1:F:521:GLY:N	1:F:538:HIS:HE2	2.11	0.48
1:B:626:THR:CG2	5:B:802:HOH:O	2.62	0.48
1:B:604:TRP:HH2	1:B:628:LEU:HB3	1.77	0.48
1:D:544:ASN:HB2	1:D:568:GLU:OE1	2.13	0.48
1:E:583:ILE:O	1:E:587:ASN:ND2	2.28	0.48
1:A:611:ARG:NH1	1:A:621:ARG:O	2.46	0.48
1:E:525:HIS:NE2	1:E:526:ASN:OD1	2.46	0.48
1:A:620:TRP:CH2	1:F:500:LEU:HD21	2.49	0.47
1:D:533:CYS:CB	1:D:563:CYS:SG	2.94	0.47
1:B:523:PHE:CE2	1:B:554:MET:HE1	2.47	0.47
1:B:671:LEU:CD1	1:B:677:LEU:HD23	2.44	0.47
1:F:539:THR:HG22	1:F:545:PHE:CD2	2.49	0.47
1:C:611:ARG:NH2	5:C:808:HOH:O	2.48	0.47
1:D:676:GLU:O	1:D:681:LEU:HD12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:PHE:CD2	1:E:606:PHE:C	2.92	0.47
1:F:617:CYS:HB3	1:F:620:TRP:CD1	2.43	0.47
1:F:680:GLU:CB	5:F:830:HOH:O	2.62	0.47
1:B:523:PHE:CZ	1:B:663:PRO:HG3	2.50	0.46
1:A:513:ILE:H	1:A:513:ILE:HG13	1.59	0.46
1:F:515:CYS:SG	1:F:516:TYR:N	2.89	0.46
1:E:598:HIS:CD2	1:E:601:ASN:CG	2.93	0.46
1:D:512:GLN:HG3	1:D:520:PRO:HB3	1.96	0.46
1:E:569:PHE:HD1	5:E:804:HOH:O	1.99	0.46
1:E:550:LEU:HD21	1:E:610:GLN:CG	2.45	0.46
1:F:543:GLN:HB2	1:F:568:GLU:OE1	2.15	0.46
1:D:515:CYS:O	1:D:517:CYS:N	2.48	0.46
1:C:560:CYS:SG	1:C:563:CYS:HB2	2.56	0.46
1:D:564:ASN:ND2	1:D:567:ILE:O	2.49	0.46
1:D:650:LYS:N	5:D:801:HOH:O	2.18	0.46
1:E:588:LEU:HB3	1:E:597:HIS:CD2	2.51	0.46
1:E:554:MET:HB2	1:E:666:ILE:CD1	2.46	0.46
1:A:559:CYS:HB3	1:A:569:PHE:HB3	1.98	0.45
1:A:598:HIS:HB3	1:A:601:ASN:HB2	1.97	0.45
1:A:665:HIS:HB3	5:A:844:HOH:O	2.16	0.45
1:A:616:ILE:HD12	1:A:620:TRP:HB3	1.98	0.45
1:D:549:LEU:N	1:D:549:LEU:CD1	2.80	0.45
1:D:577:TRP:CZ2	1:D:628:LEU:HD11	2.50	0.45
1:C:550:LEU:HD11	1:C:610:GLN:HG2	1.98	0.45
1:C:611:ARG:NH2	5:C:810:HOH:O	2.50	0.45
1:F:598:HIS:CD2	1:F:601:ASN:OD1	2.70	0.44
1:F:682:LEU:CD1	1:F:690:LEU:HD11	2.48	0.44
1:A:554:MET:HB2	1:A:666:ILE:HD12	1.98	0.44
1:C:542:MET:HE2	1:C:558:PHE:CE1	2.52	0.44
1:D:559:CYS:SG	1:D:677:LEU:HD11	2.58	0.44
1:E:527:MET:HB3	1:E:527:MET:HE2	1.72	0.44
1:E:598:HIS:CD2	1:E:601:ASN:OD1	2.70	0.44
1:E:525:HIS:CD2	1:E:526:ASN:OD1	2.70	0.44
1:E:556:PHE:HE1	1:E:572:ARG:HD2	1.81	0.44
1:F:501:SER:O	1:F:505:LYS:HG2	2.17	0.44
1:A:681:LEU:HD21	5:A:816:HOH:O	2.17	0.44
1:D:567:ILE:HD11	1:E:606:PHE:HD1	1.72	0.44
1:E:525:HIS:CE1	1:E:526:ASN:OD1	2.70	0.44
1:F:616:ILE:CG1	5:F:807:HOH:O	2.50	0.44
1:F:599:LEU:HD12	1:F:599:LEU:O	2.18	0.44
1:F:608:LEU:HA	1:F:608:LEU:HD23	1.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:616:ILE:CG2	1:F:617:CYS:N	2.81	0.43
1:F:546:LYS:CB	5:F:833:HOH:O	2.66	0.43
1:A:598:HIS:CE1	1:A:600:LEU:HB3	2.53	0.43
1:A:618:GLU:CB	5:A:851:HOH:O	2.66	0.43
1:C:561:THR:HG22	1:C:566:GLY:C	2.43	0.43
1:C:588:LEU:O	1:C:592:GLN:HG2	2.19	0.43
1:D:610:GLN:O	1:D:613:GLN:HB2	2.18	0.43
1:E:581:LEU:HD13	1:E:636:LEU:HG	1.99	0.43
1:F:538:HIS:HB2	1:F:541:CYS:CB	2.48	0.43
1:C:561:THR:HG22	1:C:567:ILE:CA	2.49	0.43
1:F:584:ALA:HA	1:F:606:PHE:CE2	2.54	0.43
1:D:598:HIS:HB3	1:D:601:ASN:HB2	2.01	0.43
1:C:598:HIS:HB3	1:C:601:ASN:HB2	2.00	0.43
1:F:604:TRP:HZ2	1:F:608:LEU:HD11	1.66	0.43
1:A:675:GLU:HG2	5:A:816:HOH:O	2.19	0.42
1:B:515:CYS:SG	1:B:516:TYR:N	2.91	0.42
1:E:523:PHE:CG	1:E:524:ASP:N	2.87	0.42
1:D:548:LYS:C	1:D:549:LEU:HD12	2.43	0.42
1:D:676:GLU:O	1:D:681:LEU:CD1	2.67	0.42
1:B:669:VAL:O	3:B:704:EDO:H21	2.19	0.42
1:E:542:MET:HE2	1:E:545:PHE:CD2	2.51	0.42
1:B:647:ARG:HA	1:B:653:PRO:HA	2.00	0.42
1:E:573:MET:HA	1:E:690:LEU:CD2	2.43	0.42
1:B:569:PHE:CZ	1:B:571:ARG:HG3	2.55	0.42
1:E:604:TRP:N	1:E:605:PRO:CD	2.82	0.42
1:C:595:LYS:HG3	1:C:596:TYR:CD2	2.54	0.42
1:D:571:ARG:NH2	1:D:679:ASP:OD2	2.53	0.42
1:E:539:THR:HA	1:E:542:MET:SD	2.59	0.42
1:B:660:HIS:HD2	5:B:834:HOH:O	2.02	0.42
1:A:515:CYS:SG	1:A:516:TYR:N	2.93	0.41
1:A:564:ASN:ND2	1:A:567:ILE:O	2.46	0.41
1:A:620:TRP:CE3	1:A:620:TRP:CA	3.01	0.41
1:E:533:CYS:CB	1:E:563:CYS:SG	2.92	0.41
1:E:543:GLN:N	1:E:568:GLU:OE2	2.52	0.41
1:E:550:LEU:HD21	1:E:610:GLN:HG3	2.01	0.41
1:D:640:SER:O	1:D:659:ARG:NH1	2.52	0.41
1:B:674:HIS:HE1	5:F:812:HOH:O	2.02	0.41
1:D:542:MET:HE2	1:D:542:MET:HB3	2.00	0.41
1:F:603:ILE:O	1:F:607:ILE:HG13	2.21	0.41
1:B:605:PRO:O	1:B:608:LEU:HG	2.20	0.41
1:B:542:MET:HE3	1:B:558:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:CYS:O	1:C:534:ARG:HB2	2.21	0.41
1:C:614:LEU:HD23	1:C:614:LEU:HA	1.90	0.41
1:D:539:THR:HG23	1:D:545:PHE:CD2	2.56	0.41
1:E:523:PHE:CD2	1:E:554:MET:HE1	2.56	0.41
1:F:620:TRP:O	1:F:623:LEU:CB	2.69	0.41
1:B:576:GLU:HB3	1:B:578:VAL:HG12	2.02	0.41
1:A:539:THR:O	1:A:542:MET:HB2	2.20	0.41
1:E:523:PHE:CZ	1:E:663:PRO:HG3	2.55	0.41
1:A:553:ASP:CG	1:A:572:ARG:HH22	2.28	0.40
1:C:556:PHE:CE2	1:C:572:ARG:HD2	2.56	0.40
1:F:636:LEU:HD13	1:F:656:TYR:CG	2.56	0.40
1:B:543:GLN:OE1	1:C:609:GLU:CG	2.61	0.40
1:C:527:MET:HE2	1:C:536:TRP:HB3	2.02	0.40
1:C:555:PHE:HB3	1:C:573:MET:HB2	2.03	0.40
1:E:542:MET:HG3	1:E:545:PHE:HB2	2.01	0.40
1:F:691:MET:HA	1:F:692:PRO:HD3	1.91	0.40
1:C:567:ILE:HD13	1:C:567:ILE:HA	1.88	0.40
1:D:591:HIS:ND1	1:D:591:HIS:N	2.69	0.40
1:F:503:ASP:N	1:F:503:ASP:OD1	2.52	0.40
1:F:543:GLN:HE21	1:F:561:THR:CG2	2.25	0.40

All (5) 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)
5:C:844:HOH:O	5:F:825:HOH:O[1_545]	0.39	1.81
5:D:819:HOH:O	5:D:823:HOH:O[2_556]	0.53	1.67
5:C:812:HOH:O	5:F:809:HOH:O[1_545]	0.54	1.66
5:C:841:HOH:O	5:F:828:HOH:O[1_545]	0.72	1.48
1:C:611:ARG:NH1	1:F:503:ASP:O[4_445]	1.94	0.26

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	178/209 (85%)	175 (98%)	3 (2%)	0	100	100
1	B	182/209 (87%)	179 (98%)	3 (2%)	0	100	100
1	C	188/209 (90%)	185 (98%)	3 (2%)	0	100	100
1	D	183/209 (88%)	178 (97%)	5 (3%)	0	100	100
1	E	170/209 (81%)	167 (98%)	3 (2%)	0	100	100
1	F	188/209 (90%)	184 (98%)	4 (2%)	0	100	100
All	All	1089/1254 (87%)	1068 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	148/196 (76%)	142 (96%)	6 (4%)	27	38
1	B	150/196 (76%)	148 (99%)	2 (1%)	61	72
1	C	155/196 (79%)	150 (97%)	5 (3%)	34	46
1	D	149/196 (76%)	147 (99%)	2 (1%)	61	72
1	E	118/196 (60%)	115 (98%)	3 (2%)	42	54
1	F	144/196 (74%)	140 (97%)	4 (3%)	38	51
All	All	864/1176 (74%)	842 (98%)	22 (2%)	42	54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	LYS
1	B	620	TRP
1	A	513	ILE
1	A	539	THR
1	A	572	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	GLU
1	A	611	ARG
1	A	620	TRP
1	C	534	ARG
1	C	572	ARG
1	C	594	GLN
1	C	611	ARG
1	C	672	GLU
1	D	572	ARG
1	D	591	HIS
1	E	602	ASP
1	E	607	ILE
1	E	610	GLN
1	F	507	ARG
1	F	549	LEU
1	F	572	ARG
1	F	578	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	610	GLN
1	B	634	GLN
1	B	665	HIS
1	A	525	HIS
1	A	543	GLN
1	A	665	HIS
1	C	525	HIS
1	C	592	GLN
1	C	610	GLN
1	C	612	HIS
1	C	660	HIS
1	C	665	HIS
1	D	526	ASN
1	D	544	ASN
1	D	660	HIS
1	D	665	HIS
1	E	598	HIS
1	E	660	HIS
1	F	543	GLN
1	F	598	HIS
1	F	610	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	674	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
4	PO4	D	703	-	4,4,4	0.97	0	6,6,6	0.46	0
3	EDO	C	704	-	3,3,3	0.43	0	2,2,2	0.38	0
3	EDO	B	704	-	3,3,3	0.38	0	2,2,2	0.37	0
4	PO4	C	703	-	4,4,4	0.97	0	6,6,6	0.46	0
3	EDO	B	703	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	F	703	-	3,3,3	0.40	0	2,2,2	0.41	0
3	EDO	C	705	-	3,3,3	0.33	0	2,2,2	0.35	0

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	EDO	C	704	-	-	0/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	F	703	-	-	0/1/1/1	-
3	EDO	C	705	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	705	EDO	O1-C1-C2-O2
3	B	704	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	704	EDO	4	0
3	B	704	EDO	6	0
3	F	703	EDO	1	0
3	C	705	EDO	2	0

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

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	184/209 (88%)	0.53	8 (4%) 40 37	28, 66, 92, 121	0
1	B	186/209 (88%)	0.61	13 (6%) 22 19	28, 67, 103, 131	0
1	C	192/209 (91%)	0.78	23 (11%) 9 7	33, 71, 116, 134	0
1	D	187/209 (89%)	0.80	11 (5%) 28 25	42, 79, 112, 119	0
1	E	180/209 (86%)	1.16	26 (14%) 6 4	51, 96, 128, 135	0
1	F	192/209 (91%)	1.18	34 (17%) 4 2	28, 86, 127, 143	0
All	All	1121/1254 (89%)	0.84	115 (10%) 12 9	28, 76, 119, 143	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	514	TYR	5.0
1	C	513	ILE	4.5
1	D	567	ILE	4.4
1	E	525	HIS	4.2
1	B	622	THR	4.2
1	F	649	PHE	3.8
1	D	508	VAL	3.6
1	C	564	ASN	3.6
1	B	649	PHE	3.6
1	A	593	HIS	3.5
1	E	537	PHE	3.4
1	F	521	GLY	3.4
1	F	541	CYS	3.3
1	E	615	PRO	3.3
1	F	688	LEU	3.3
1	C	614	LEU	3.3
1	F	604	TRP	3.3
1	B	513	ILE	3.3
1	E	649	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	528	LEU	3.2
1	F	625	GLU	3.1
1	C	567	ILE	3.1
1	E	565	ASN	3.1
1	F	628	LEU	3.0
1	B	525	HIS	3.0
1	C	520	PRO	3.0
1	E	682	LEU	3.0
1	E	516	TYR	2.9
1	C	544	ASN	2.8
1	F	591	HIS	2.8
1	F	500	LEU	2.8
1	F	654	ALA	2.8
1	E	550	LEU	2.8
1	C	518	GLY	2.8
1	C	613	GLN	2.8
1	F	618	GLU	2.8
1	D	558	PHE	2.8
1	F	678	SER	2.7
1	C	557	VAL	2.7
1	F	520	PRO	2.7
1	F	615	PRO	2.7
1	D	614	LEU	2.7
1	B	648	GLU	2.7
1	E	623	LEU	2.6
1	E	521	GLY	2.6
1	B	616	ILE	2.6
1	D	644	VAL	2.6
1	E	543	GLN	2.6
1	F	567	ILE	2.6
1	F	681	LEU	2.6
1	F	626	THR	2.6
1	F	590	LYS	2.6
1	D	516	TYR	2.6
1	E	514	TYR	2.6
1	A	612	HIS	2.5
1	E	567	ILE	2.5
1	A	508	VAL	2.5
1	E	523	PHE	2.5
1	E	690	LEU	2.5
1	F	624	PRO	2.4
1	B	549	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	591	HIS	2.4
1	B	514	TYR	2.4
1	C	516	TYR	2.4
1	E	528	LEU	2.4
1	B	545	PHE	2.4
1	D	615	PRO	2.4
1	A	595	LYS	2.4
1	D	688	LEU	2.4
1	F	682	LEU	2.4
1	C	559	CYS	2.4
1	F	607	ILE	2.3
1	B	591	HIS	2.3
1	E	541	CYS	2.3
1	E	504	GLU	2.3
1	E	693	GLU	2.3
1	C	673	PRO	2.3
1	C	688	LEU	2.3
1	C	693	GLU	2.3
1	F	627	ALA	2.3
1	C	610	GLN	2.3
1	A	622	THR	2.3
1	A	592	GLN	2.2
1	C	566	GLY	2.2
1	B	546	LYS	2.2
1	F	614	LEU	2.2
1	C	536	TRP	2.2
1	C	569	PHE	2.2
1	C	527	MET	2.2
1	E	513	ILE	2.2
1	F	616	ILE	2.2
1	B	650	LYS	2.2
1	D	645	CYS	2.2
1	F	589	ARG	2.2
1	F	655	PHE	2.2
1	F	611	ARG	2.2
1	F	620	TRP	2.2
1	E	558	PHE	2.2
1	A	689	MET	2.1
1	E	614	LEU	2.1
1	B	523	PHE	2.1
1	A	523	PHE	2.1
1	C	523	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	629	MET	2.1
1	D	657	ALA	2.1
1	F	601	ASN	2.1
1	F	525	HIS	2.1
1	F	575	ILE	2.1
1	F	630	GLU	2.1
1	E	679	ASP	2.1
1	C	558	PHE	2.1
1	C	616	ILE	2.1
1	D	560	CYS	2.1
1	E	571	ARG	2.0
1	E	510	GLU	2.0

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](#)

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
3	EDO	C	704	4/4	0.74	0.15	79,82,84,95	0
3	EDO	C	705	4/4	0.78	0.15	72,76,78,81	0
3	EDO	F	703	4/4	0.79	0.17	79,81,89,90	0
3	EDO	B	704	4/4	0.90	0.14	64,65,69,70	0
2	ZN	F	701	1/1	0.91	0.08	103,103,103,103	0
4	PO4	C	703	5/5	0.91	0.12	61,62,80,81	0
4	PO4	D	703	5/5	0.92	0.18	55,64,75,77	0
2	ZN	C	702	1/1	0.95	0.06	95,95,95,95	0
2	ZN	C	701	1/1	0.95	0.08	104,104,104,104	0
3	EDO	B	703	4/4	0.95	0.18	43,44,49,55	0
2	ZN	D	702	1/1	0.96	0.07	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	E	701	1/1	0.97	0.04	121,121,121,121	0
2	ZN	E	702	1/1	0.97	0.05	89,89,89,89	0
2	ZN	D	701	1/1	0.98	0.04	102,102,102,102	0
2	ZN	A	702	1/1	0.98	0.03	46,46,46,46	0
2	ZN	B	702	1/1	0.98	0.03	35,35,35,35	0
2	ZN	A	701	1/1	0.98	0.04	61,61,61,61	0
2	ZN	F	702	1/1	0.99	0.05	68,68,68,68	0
2	ZN	B	701	1/1	1.00	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.