



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:19 AM UTC

PDB ID : 1B09 / pdb_00001b09
Title : HUMAN C-REACTIVE PROTEIN COMPLEXED WITH PHOSPHO-CHOLINE
Authors : Thompson, D.; Pepys, M.B.; Wood, S.P.
Deposited on : 1998-11-18
Resolution : 2.50 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

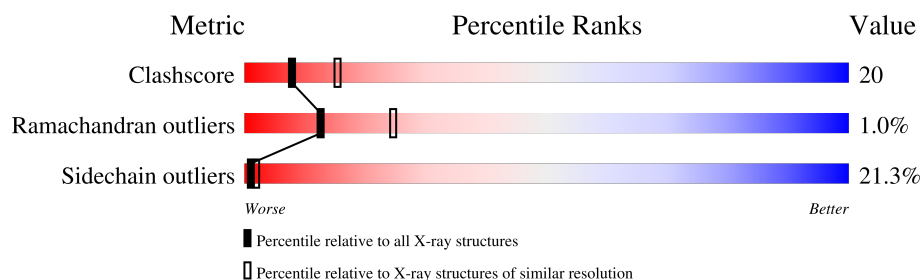
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	
1	B	206	
1	C	206	
1	D	206	
1	E	206	

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
3	PC	A	500	-	X	-	-
3	PC	C	500	-	X	-	-
3	PC	D	500	-	X	-	-
3	PC	E	500	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8225 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.

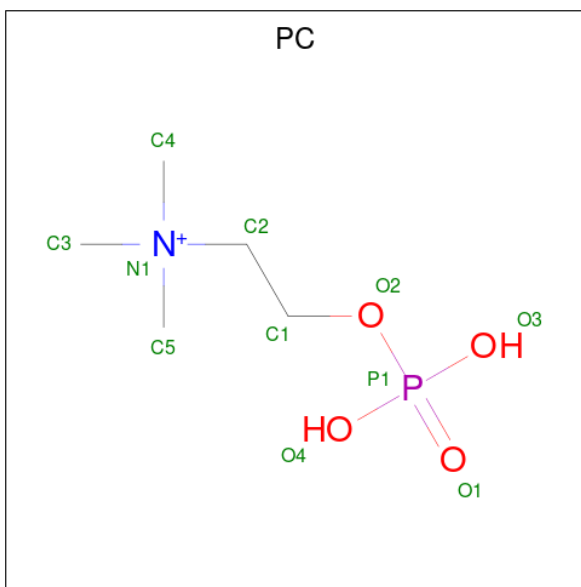
- Molecule 1 is a protein called PROTEIN (C-REACTIVE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	B	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	C	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	D	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			
1	E	206	Total	C	N	O	S	0	0	0
			1632	1058	261	309	4			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is PHOSPHOCHOLINE (CCD ID: PC) (formula: C₅H₁₅NO₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
3	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
3	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
3	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
3	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

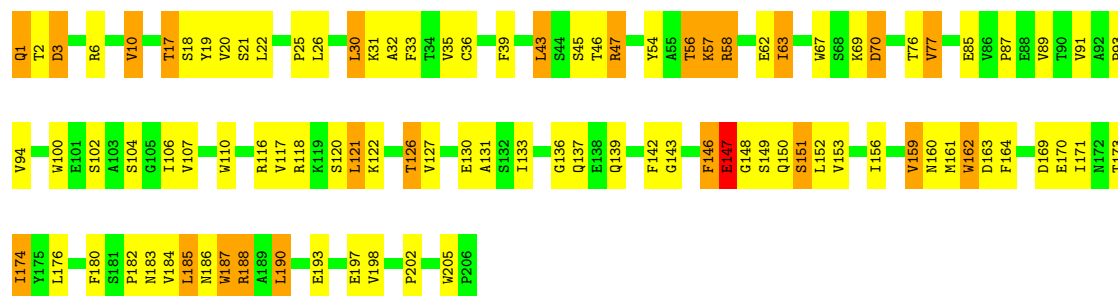
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

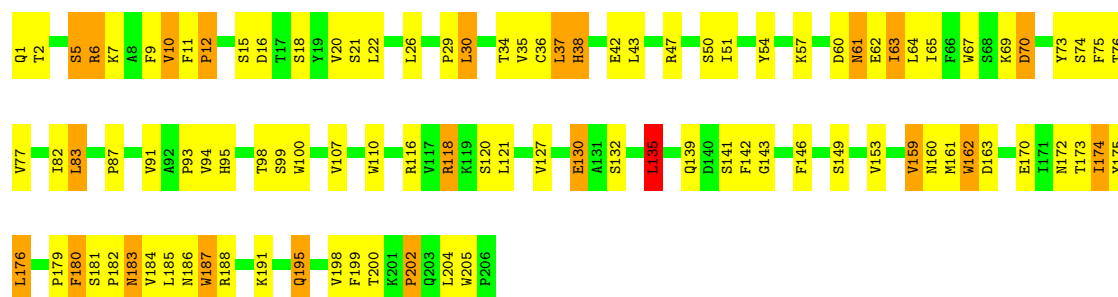
• Molecule 1: PROTEIN (C-REACTIVE PROTEIN)

Chain A: 

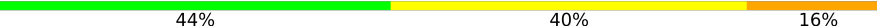


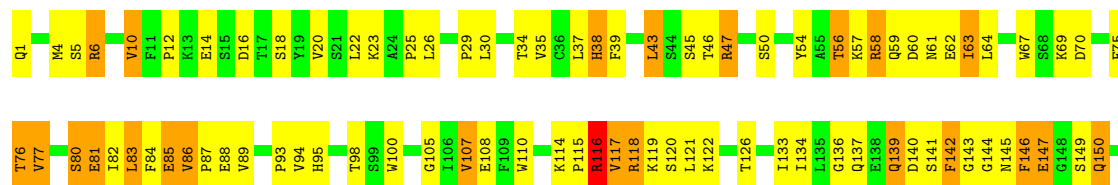
• Molecule 1: PROTEIN (C-REACTIVE PROTEIN)

Chain B: 



• Molecule 1: PROTEIN (C-REACTIVE PROTEIN)

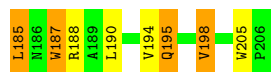
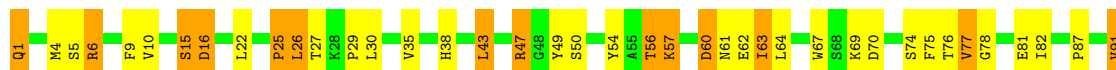
Chain C: 





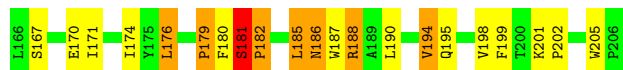
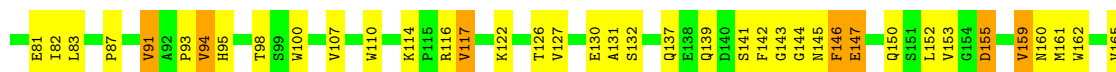
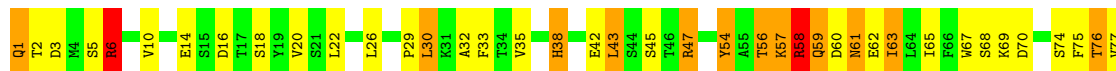
• Molecule 1: PROTEIN (C-REACTIVE PROTEIN)

Chain D: 56% 31% 13%



• Molecule 1: PROTEIN (C-REACTIVE PROTEIN)

Chain E: 51% 34% 13%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	193.94Å 193.94Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.6 (20.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8225	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.35	7/1678 (0.4%)	1.54	13/2279 (0.6%)
1	B	1.34	7/1678 (0.4%)	1.55	19/2279 (0.8%)
1	C	1.36	9/1678 (0.5%)	1.60	15/2279 (0.7%)
1	D	1.35	8/1678 (0.5%)	1.53	16/2279 (0.7%)
1	E	1.29	6/1678 (0.4%)	1.60	22/2279 (1.0%)
All	All	1.34	37/8390 (0.4%)	1.57	85/11395 (0.7%)

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	C	0	1
1	E	0	1
All	All	0	3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	TRP	NE1-CE2	10.28	1.48	1.37
1	E	162	TRP	NE1-CE2	10.14	1.48	1.37
1	A	162	TRP	NE1-CE2	10.13	1.48	1.37
1	C	110	TRP	NE1-CE2	10.13	1.48	1.37
1	C	187	TRP	NE1-CE2	10.13	1.48	1.37
1	B	187	TRP	NE1-CE2	10.12	1.48	1.37
1	A	67	TRP	NE1-CE2	10.11	1.48	1.37
1	C	67	TRP	NE1-CE2	10.10	1.48	1.37
1	E	110	TRP	NE1-CE2	10.10	1.48	1.37
1	D	100	TRP	NE1-CE2	10.09	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	TRP	NE1-CE2	10.06	1.48	1.37
1	B	162	TRP	NE1-CE2	10.04	1.48	1.37
1	C	205	TRP	NE1-CE2	10.04	1.48	1.37
1	A	110	TRP	NE1-CE2	10.04	1.48	1.37
1	C	100	TRP	NE1-CE2	10.02	1.48	1.37
1	B	110	TRP	NE1-CE2	10.01	1.48	1.37
1	E	67	TRP	NE1-CE2	9.98	1.48	1.37
1	B	100	TRP	NE1-CE2	9.97	1.48	1.37
1	D	67	TRP	NE1-CE2	9.95	1.48	1.37
1	B	67	TRP	NE1-CE2	9.93	1.48	1.37
1	D	205	TRP	NE1-CE2	9.91	1.48	1.37
1	D	187	TRP	NE1-CE2	9.89	1.48	1.37
1	E	100	TRP	NE1-CE2	9.88	1.48	1.37
1	C	162	TRP	NE1-CE2	9.87	1.48	1.37
1	A	205	TRP	NE1-CE2	9.85	1.48	1.37
1	D	162	TRP	NE1-CE2	9.82	1.48	1.37
1	D	110	TRP	NE1-CE2	9.80	1.48	1.37
1	A	100	TRP	NE1-CE2	9.74	1.48	1.37
1	E	188	ARG	CZ-NH2	6.57	1.42	1.33
1	C	150	GLN	CD-OE1	6.12	1.35	1.23
1	D	144	GLY	C-O	6.03	1.27	1.23
1	E	61	ASN	CG-OD1	5.75	1.34	1.23
1	B	61	ASN	CG-OD1	5.57	1.34	1.23
1	C	61	ASN	CG-OD1	5.53	1.34	1.23
1	C	150	GLN	CD-NE2	-5.37	1.22	1.33
1	A	147	GLU	C-N	5.34	1.40	1.33
1	D	61	ASN	CG-OD1	5.32	1.33	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	GLU	O-C-N	-10.14	109.07	122.77
1	C	146	PHE	CA-C-N	9.43	136.37	121.66
1	C	146	PHE	C-N-CA	9.43	136.37	121.66
1	E	147	GLU	O-C-N	-8.44	111.37	122.59
1	B	146	PHE	CA-C-N	-7.91	111.80	122.72
1	B	146	PHE	C-N-CA	-7.91	111.80	122.72
1	C	25	PRO	N-CA-CB	7.20	107.46	102.35
1	D	16	ASP	O-C-N	7.16	130.58	122.27
1	D	180	PHE	CA-CB-CG	-6.49	107.31	113.80
1	E	146	PHE	CA-C-N	6.34	133.66	121.54
1	E	146	PHE	C-N-CA	6.34	133.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	PRO	N-CA-CB	6.11	109.00	103.19
1	A	25	PRO	N-CA-CB	6.08	107.10	102.36
1	C	179	PRO	N-CA-CB	6.04	108.95	103.33
1	A	147	GLU	O-C-N	-6.02	116.46	123.27
1	B	93	PRO	N-CA-CB	5.94	108.86	103.34
1	C	93	PRO	N-CA-CB	5.89	108.48	103.35
1	E	54	TYR	O-C-N	-5.89	115.35	123.12
1	E	181	SER	CA-C-O	5.79	126.69	120.08
1	E	186	ASN	N-CA-C	5.79	118.62	107.44
1	C	29	PRO	N-CA-CB	5.75	108.35	103.35
1	A	3	ASP	CA-CB-CG	-5.70	106.91	112.60
1	A	17	THR	O-C-N	-5.67	114.84	122.22
1	A	6	ARG	CD-NE-CZ	-5.63	116.51	124.40
1	A	70	ASP	N-CA-CB	-5.61	107.77	114.17
1	A	202	PRO	N-CA-CB	5.59	108.22	103.35
1	B	180	PHE	CA-CB-CG	-5.56	108.24	113.80
1	B	34	THR	CA-C-N	-5.53	115.43	123.06
1	B	34	THR	C-N-CA	-5.53	115.43	123.06
1	C	85	GLU	CA-C-N	-5.52	117.17	123.25
1	C	85	GLU	C-N-CA	-5.52	117.17	123.25
1	A	93	PRO	N-CA-CB	5.50	108.44	103.33
1	E	201	LYS	CA-C-N	5.50	125.25	119.76
1	E	201	LYS	C-N-CA	5.50	125.25	119.76
1	C	116	ARG	CD-NE-CZ	-5.46	116.75	124.40
1	C	58	ARG	CD-NE-CZ	-5.43	116.79	124.40
1	D	188	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	B	179	PRO	N-CA-CB	5.41	108.45	102.72
1	A	146	PHE	O-C-N	5.39	129.41	123.16
1	B	118	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	E	182	PRO	CA-C-N	-5.36	113.19	122.14
1	E	182	PRO	C-N-CA	-5.36	113.19	122.14
1	D	145	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	116	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	C	180	PHE	CA-CB-CG	-5.28	108.52	113.80
1	E	58	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	B	202	PRO	N-CA-CB	5.27	107.94	103.35
1	A	188	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	B	188	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	D	47	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	E	93	PRO	N-CA-CB	5.26	107.99	103.31
1	D	25	PRO	N-CA-CB	5.26	107.69	102.17
1	E	202	PRO	N-CA-CB	5.24	108.21	103.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	CA-C-N	-5.18	117.81	123.30
1	B	135	LEU	C-N-CA	-5.18	117.81	123.30
1	D	29	PRO	N-CA-CB	5.17	108.14	103.33
1	B	12	PRO	N-CA-CB	5.15	108.25	103.46
1	D	6	ARG	N-CA-CB	-5.14	108.31	114.17
1	D	165	VAL	N-CA-C	5.14	114.98	107.37
1	C	202	PRO	N-CA-CB	5.13	107.88	103.31
1	E	180	PHE	CA-C-N	-5.13	115.77	122.74
1	E	180	PHE	C-N-CA	-5.13	115.77	122.74
1	B	47	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	133	ILE	CA-C-N	-5.10	115.85	122.94
1	A	133	ILE	C-N-CA	-5.10	115.85	122.94
1	E	29	PRO	N-CA-CB	5.08	108.08	103.15
1	E	6	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	B	70	ASP	CA-C-N	-5.08	118.00	122.97
1	B	70	ASP	C-N-CA	-5.08	118.00	122.97
1	C	118	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	C	6	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	D	9	PHE	CA-C-N	-5.07	116.50	123.14
1	D	9	PHE	C-N-CA	-5.07	116.50	123.14
1	E	179	PRO	O-C-N	-5.07	117.08	123.21
1	D	6	ARG	CD-NE-CZ	-5.05	117.34	124.40
1	D	93	PRO	N-CA-CB	5.04	108.02	103.33
1	E	194	VAL	CA-CB-CG1	5.04	118.97	110.40
1	D	180	PHE	CA-C-N	-5.04	116.71	122.26
1	D	180	PHE	C-N-CA	-5.04	116.71	122.26
1	E	201	LYS	O-C-N	-5.03	118.49	121.71
1	E	199	PHE	N-CA-C	5.03	117.50	109.81
1	B	6	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	E	47	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	A	58	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	B	29	PRO	N-CA-CB	5.01	108.10	103.39

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLU	Mainchain
1	C	16	ASP	Peptide
1	E	179	PRO	Mainchain

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	1632	0	1593	68	0
1	B	1632	0	1593	58	0
1	C	1632	0	1593	75	0
1	D	1632	0	1593	56	0
1	E	1632	0	1593	68	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	11	0	13	0	0
3	B	11	0	13	0	0
3	C	11	0	13	3	0
3	D	11	0	13	2	0
3	E	11	0	13	0	0
All	All	8225	0	8030	319	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 20.

All (319) 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:85:GLU:O	1:A:116:ARG:NH2	1.90	1.05
1:B:37:LEU:HD23	1:B:37:LEU:O	1.65	0.95
1:E:130:GLU:O	1:E:130:GLU:HG3	1.65	0.93
1:A:148:GLY:O	1:A:151:SER:HB2	1.71	0.90
1:D:35:VAL:HG12	1:D:98:THR:HG22	1.53	0.90
1:B:63:ILE:HG13	1:B:63:ILE:O	1.72	0.88
1:B:37:LEU:HD23	1:B:37:LEU:C	1.98	0.88
1:E:59:GLN:NE2	1:E:61:ASN:H	1.71	0.88
1:D:1:GLN:CD	1:D:1:GLN:H3	1.82	0.88
1:E:147:GLU:HG2	1:E:150:GLN:HG3	1.55	0.88
1:B:159:VAL:HG13	1:B:187:TRP:CZ3	2.09	0.87
1:E:59:GLN:HE21	1:E:59:GLN:C	1.83	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASN:HD21	1:A:187:TRP:H	1.23	0.85
1:C:85:GLU:O	1:C:116:ARG:NH2	2.09	0.85
1:B:172:ASN:O	1:B:176:LEU:HD22	1.78	0.82
1:C:161:MET:HB2	1:C:185:LEU:HB2	1.62	0.82
1:A:69:LYS:O	1:A:70:ASP:HB2	1.78	0.81
1:A:54:TYR:HB3	1:A:63:ILE:HG23	1.64	0.80
1:B:5:SER:O	1:B:6:ARG:HB2	1.83	0.79
1:C:107:VAL:HG23	1:C:119:LYS:O	1.82	0.78
1:C:62:GLU:OE1	1:C:62:GLU:HA	1.83	0.78
1:D:155:ASP:OD1	1:D:155:ASP:N	2.16	0.78
1:E:1:GLN:H3	1:E:1:GLN:NE2	1.82	0.78
1:C:162:TRP:NE1	1:C:182:PRO:HA	2.00	0.77
1:E:59:GLN:HE22	1:E:61:ASN:H	1.32	0.76
1:E:1:GLN:NE2	1:E:1:GLN:N	2.33	0.76
1:D:1:GLN:CD	1:D:1:GLN:N	2.43	0.75
1:C:144:GLY:HA2	1:C:146:PHE:CE1	2.23	0.74
1:E:59:GLN:NE2	1:E:59:GLN:C	2.46	0.74
1:D:62:GLU:O	1:D:77:VAL:HA	1.86	0.73
1:C:43:LEU:HD21	1:C:153:VAL:HG23	1.70	0.72
1:C:183:ASN:ND2	1:C:184:VAL:HG23	2.03	0.72
1:C:170:GLU:O	1:C:174:ILE:HG12	1.89	0.72
1:B:37:LEU:C	1:B:37:LEU:CD2	2.61	0.72
1:A:30:LEU:HB2	1:A:127:VAL:HB	1.72	0.71
1:B:37:LEU:O	1:B:37:LEU:CD2	2.39	0.71
1:D:161:MET:HB3	1:D:185:LEU:HB2	1.72	0.71
1:B:202:PRO:O	1:C:118:ARG:NH2	2.22	0.70
1:C:37:LEU:O	1:C:37:LEU:HD12	1.92	0.70
1:D:56:THR:HG23	1:D:130:GLU:O	1.91	0.70
1:A:160:ASN:ND2	1:A:187:TRP:H	1.90	0.69
1:E:56:THR:HG22	1:E:58:ARG:H	1.55	0.69
1:E:75:PHE:O	1:E:82:ILE:HG22	1.93	0.69
1:C:63:ILE:HG13	1:C:63:ILE:O	1.92	0.69
1:A:186:ASN:C	1:A:186:ASN:HD22	1.99	0.69
1:D:5:SER:O	1:D:6:ARG:HB2	1.92	0.69
1:B:130:GLU:O	1:B:130:GLU:HG3	1.92	0.68
1:A:56:THR:CG2	1:A:57:LYS:N	2.57	0.68
1:E:76:THR:HB	1:E:81:GLU:HA	1.74	0.68
1:C:182:PRO:HD2	1:C:186:ASN:OD1	1.93	0.68
1:A:1:GLN:OE1	1:A:1:GLN:N	2.26	0.68
1:C:38:HIS:NE2	1:C:95:HIS:HB2	2.08	0.68
1:C:14:GLU:CD	1:C:47:ARG:HH12	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ASN:C	1:C:186:ASN:ND2	2.52	0.67
1:A:56:THR:HG22	1:A:58:ARG:H	1.60	0.67
1:D:54:TYR:HB3	1:D:63:ILE:HG23	1.78	0.66
1:E:130:GLU:O	1:E:130:GLU:CG	2.40	0.66
1:C:186:ASN:C	1:C:186:ASN:HD22	2.02	0.65
1:D:180:PHE:N	1:D:180:PHE:CD1	2.64	0.65
1:E:161:MET:HB3	1:E:185:LEU:HB2	1.77	0.65
1:C:43:LEU:CD2	1:C:153:VAL:HG23	2.27	0.64
1:C:105:GLY:O	1:C:120:SER:HA	1.98	0.64
1:E:56:THR:HG22	1:E:58:ARG:N	2.13	0.64
1:C:183:ASN:C	1:C:183:ASN:HD22	2.04	0.64
1:E:144:GLY:HA2	1:E:146:PHE:CE1	2.33	0.64
1:B:175:TYR:CD2	1:B:176:LEU:HD13	2.33	0.64
1:C:201:LYS:HB2	1:D:118:ARG:HH12	1.62	0.64
1:B:69:LYS:O	1:B:70:ASP:HB2	1.98	0.63
1:C:144:GLY:O	1:C:145:ASN:HB2	1.99	0.63
1:D:130:GLU:O	1:D:130:GLU:HG3	1.99	0.63
1:B:180:PHE:CD1	1:B:180:PHE:N	2.66	0.63
1:C:86:VAL:HG12	1:C:86:VAL:O	1.97	0.62
1:C:183:ASN:HD22	1:C:184:VAL:N	1.97	0.62
1:A:126:THR:HG22	1:A:126:THR:O	1.99	0.62
1:B:162:TRP:NE1	1:B:182:PRO:HA	2.15	0.62
1:E:59:GLN:NE2	1:E:60:ASP:N	2.47	0.62
1:C:20:VAL:HG22	1:C:194:VAL:HG23	1.81	0.62
1:E:152:LEU:HD12	1:E:153:VAL:N	2.16	0.61
1:B:160:ASN:HD21	1:B:187:TRP:H	1.49	0.61
1:D:160:ASN:ND2	1:D:187:TRP:H	1.99	0.61
1:D:160:ASN:HD21	1:D:187:TRP:H	1.49	0.61
1:A:182:PRO:HB2	1:A:185:LEU:O	2.00	0.61
1:B:130:GLU:O	1:B:130:GLU:CG	2.49	0.60
1:E:155:ASP:N	1:E:155:ASP:OD1	2.34	0.60
1:E:1:GLN:N	1:E:1:GLN:HE21	2.00	0.60
1:A:62:GLU:OE1	1:A:62:GLU:HA	2.03	0.59
1:A:121:LEU:HD23	1:A:122:LYS:N	2.17	0.59
1:D:54:TYR:CB	1:D:63:ILE:HG23	2.32	0.59
1:B:37:LEU:N	1:B:37:LEU:HD22	2.17	0.59
1:C:10:VAL:O	1:C:12:PRO:HD3	2.03	0.59
1:A:54:TYR:CB	1:A:63:ILE:HG23	2.34	0.58
1:C:136:GLY:C	1:C:137:GLN:HG2	2.27	0.58
1:E:54:TYR:HB3	1:E:63:ILE:HG23	1.85	0.58
1:A:1:GLN:N	1:A:1:GLN:CD	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ASN:ND2	1:C:188:ARG:H	2.01	0.58
1:A:121:LEU:HD23	1:A:122:LYS:H	1.69	0.58
1:A:164:PHE:N	1:A:164:PHE:CD1	2.71	0.58
1:C:69:LYS:O	1:C:70:ASP:HB2	2.03	0.58
1:C:77:VAL:HG13	1:C:121:LEU:HD23	1.85	0.58
1:B:184:VAL:HG12	1:B:185:LEU:HD13	1.86	0.58
1:E:59:GLN:NE2	1:E:61:ASN:N	2.48	0.58
1:A:33:PHE:CD1	1:A:33:PHE:C	2.82	0.57
1:A:32:ALA:O	1:A:33:PHE:HB3	2.05	0.57
1:C:186:ASN:HD22	1:C:189:ALA:H	1.53	0.57
1:E:65:ILE:HD11	1:E:98:THR:HG21	1.85	0.57
1:C:200:THR:HG22	1:C:200:THR:O	2.04	0.57
1:A:137:GLN:NE2	1:A:146:PHE:HB3	2.21	0.56
1:C:163:ASP:H	1:C:183:ASN:HD21	1.52	0.56
1:E:56:THR:CG2	1:E:57:LYS:N	2.68	0.56
1:D:139:GLN:NE2	1:D:143:GLY:H	2.03	0.56
1:A:130:GLU:HG3	1:A:130:GLU:O	2.06	0.56
1:A:136:GLY:O	1:A:137:GLN:HG2	2.05	0.56
1:B:42:GLU:HG3	1:C:117:VAL:HG21	1.89	0.55
1:C:54:TYR:CD2	1:C:133:ILE:HG12	2.41	0.55
1:C:81:GLU:OE2	3:C:500:PC:H31	2.07	0.55
1:A:174:ILE:HD11	1:A:180:PHE:HB3	1.89	0.54
1:B:75:PHE:O	1:B:82:ILE:HG22	2.07	0.54
1:E:144:GLY:O	1:E:145:ASN:HB2	2.07	0.54
1:A:46:THR:O	1:A:69:LYS:HD2	2.08	0.54
1:A:56:THR:HG23	1:A:57:LYS:N	2.21	0.54
1:C:34:THR:HG21	1:C:166:LEU:HB2	1.90	0.54
1:D:194:VAL:CG1	1:D:198:VAL:HG13	2.37	0.54
1:A:56:THR:HG22	1:A:58:ARG:N	2.21	0.54
1:A:152:LEU:HD12	1:A:153:VAL:N	2.23	0.54
1:B:73:TYR:O	1:B:83:LEU:HD12	2.08	0.54
1:C:4:MET:O	1:C:187:TRP:NE1	2.41	0.53
1:D:91:VAL:HG12	1:D:91:VAL:O	2.08	0.53
1:D:163:ASP:OD1	1:D:163:ASP:C	2.48	0.53
1:B:160:ASN:ND2	1:B:187:TRP:H	2.05	0.53
1:D:159:VAL:CG2	1:D:159:VAL:O	2.56	0.53
1:A:186:ASN:HD22	1:A:187:TRP:N	2.06	0.53
1:B:54:TYR:CD1	1:B:63:ILE:HG23	2.44	0.53
1:A:117:VAL:HG22	1:E:42:GLU:OE2	2.09	0.53
1:A:56:THR:HG23	1:A:57:LYS:H	1.75	0.52
1:C:56:THR:HG22	1:C:59:GLN:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:C	1:A:33:PHE:HD1	2.17	0.52
1:E:91:VAL:HG22	1:E:91:VAL:O	2.09	0.52
1:D:140:ASP:HB2	1:D:145:ASN:HB3	1.92	0.52
1:E:160:ASN:ND2	1:E:187:TRP:H	2.06	0.52
1:E:59:GLN:NE2	1:E:59:GLN:CA	2.71	0.52
1:C:56:THR:HG22	1:C:58:ARG:H	1.75	0.51
1:D:157:GLY:O	1:D:158:ASN:HB2	2.11	0.51
1:C:84:PHE:CE1	1:C:119:LYS:HD2	2.44	0.51
1:D:49:TYR:N	1:D:49:TYR:CD1	2.79	0.51
1:E:18:SER:HA	1:E:195:GLN:O	2.10	0.51
1:A:18:SER:O	1:A:19:TYR:HB3	2.11	0.51
1:B:54:TYR:HD1	1:B:62:GLU:HB3	1.76	0.50
1:D:98:THR:O	1:D:98:THR:CG2	2.57	0.50
1:C:54:TYR:O	1:C:62:GLU:HB3	2.11	0.50
1:D:139:GLN:HE22	1:D:143:GLY:H	1.58	0.50
1:B:91:VAL:O	1:B:91:VAL:HG13	2.10	0.50
1:D:75:PHE:O	1:D:82:ILE:HG22	2.11	0.50
1:E:159:VAL:HG13	1:E:187:TRP:CZ3	2.47	0.50
1:D:57:LYS:HD3	1:D:130:GLU:CD	2.36	0.50
1:D:141:SER:O	1:D:142:PHE:C	2.55	0.50
1:A:170:GLU:O	1:A:174:ILE:HD12	2.11	0.50
1:B:62:GLU:HA	1:B:62:GLU:OE1	2.12	0.50
1:E:54:TYR:CZ	1:E:131:ALA:CB	2.95	0.49
1:C:183:ASN:ND2	1:C:183:ASN:C	2.67	0.49
1:C:37:LEU:HD12	1:C:37:LEU:C	2.37	0.49
1:D:144:GLY:HA2	1:D:146:PHE:CE1	2.48	0.49
1:A:139:GLN:HE21	1:A:143:GLY:HA2	1.78	0.49
1:A:18:SER:O	1:A:137:GLN:HG2	2.13	0.49
1:A:85:GLU:C	1:A:116:ARG:HH22	2.10	0.49
1:C:201:LYS:CB	1:D:118:ARG:HH12	2.26	0.49
1:D:81:GLU:CD	3:D:500:PC:H52	2.37	0.49
1:A:182:PRO:CB	1:A:185:LEU:O	2.61	0.49
1:B:161:MET:HB3	1:B:185:LEU:HB2	1.95	0.49
1:C:54:TYR:HD2	1:C:133:ILE:HG12	1.77	0.49
1:A:161:MET:CB	1:A:185:LEU:HB2	2.43	0.49
1:C:150:GLN:NE2	3:C:500:PC:O1	2.39	0.49
1:E:1:GLN:HE21	1:E:1:GLN:H1	1.61	0.49
1:A:21:SER:HB3	1:A:193:GLU:HB3	1.95	0.48
1:B:175:TYR:HD2	1:B:176:LEU:HD13	1.74	0.48
1:B:36:CYS:O	1:B:159:VAL:HA	2.13	0.48
1:D:25:PRO:O	1:D:26:LEU:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LYS:O	1:E:70:ASP:HB2	2.12	0.48
1:D:108:GLU:HG3	1:D:118:ARG:HD3	1.96	0.48
1:E:54:TYR:CB	1:E:63:ILE:HG23	2.43	0.48
1:B:9:PHE:CE2	1:B:20:VAL:HG11	2.49	0.48
1:B:18:SER:HA	1:B:195:GLN:O	2.13	0.48
1:C:108:GLU:OE2	1:C:118:ARG:NH1	2.47	0.48
1:B:204:LEU:HD22	1:C:115:PRO:HB2	1.94	0.48
1:D:162:TRP:CD1	1:D:182:PRO:HA	2.49	0.48
1:A:163:ASP:C	1:A:163:ASP:OD1	2.53	0.48
1:A:187:TRP:CE3	1:A:190:LEU:HD13	2.48	0.48
1:C:77:VAL:HG13	1:C:121:LEU:CD2	2.42	0.48
1:C:162:TRP:HA	1:C:183:ASN:ND2	2.29	0.48
1:C:162:TRP:CD1	1:C:182:PRO:HA	2.48	0.48
1:D:54:TYR:CG	1:D:63:ILE:HG23	2.49	0.48
1:A:47:ARG:NH2	1:A:151:SER:O	2.43	0.47
1:D:110:TRP:CE3	1:D:115:PRO:HB3	2.50	0.47
1:D:16:ASP:OD1	1:D:16:ASP:O	2.31	0.47
1:C:35:VAL:CG1	1:C:98:THR:HG22	2.45	0.47
1:E:2:THR:O	1:E:190:LEU:N	2.45	0.47
1:C:141:SER:O	1:C:143:GLY:N	2.48	0.47
1:A:36:CYS:O	1:A:159:VAL:HA	2.14	0.47
1:B:11:PHE:N	1:B:11:PHE:CD1	2.83	0.47
1:B:82:ILE:HB	1:B:121:LEU:HD22	1.97	0.47
1:B:176:LEU:HD13	1:B:176:LEU:N	2.30	0.47
1:B:38:HIS:NE2	1:B:95:HIS:HB2	2.31	0.46
1:B:65:ILE:HD11	1:B:98:THR:HG21	1.97	0.46
1:E:38:HIS:HB3	1:E:205:TRP:CZ2	2.50	0.46
1:B:30:LEU:HB2	1:B:127:VAL:HB	1.97	0.46
1:B:141:SER:O	1:B:143:GLY:N	2.48	0.46
1:B:10:VAL:HG13	1:B:199:PHE:HB2	1.98	0.46
1:C:161:MET:HB3	1:C:184:VAL:HB	1.97	0.46
1:C:163:ASP:N	1:C:183:ASN:HD21	2.13	0.46
1:C:167:SER:OG	1:C:170:GLU:HG3	2.16	0.46
1:B:54:TYR:O	1:B:62:GLU:HB3	2.15	0.46
1:D:1:GLN:O	1:D:1:GLN:NE2	2.49	0.46
1:E:167:SER:OG	1:E:170:GLU:HG3	2.16	0.46
1:C:161:MET:CB	1:C:185:LEU:HB2	2.39	0.46
1:D:150:GLN:NE2	3:D:500:PC:O4	2.48	0.46
1:B:199:PHE:N	1:B:199:PHE:CD1	2.83	0.46
1:C:60:ASP:OD2	1:C:140:ASP:HA	2.16	0.46
1:E:54:TYR:CG	1:E:63:ILE:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:SER:CB	1:E:139:GLN:HE22	2.29	0.46
1:A:54:TYR:CE1	1:A:131:ALA:HB2	2.51	0.45
1:B:170:GLU:O	1:B:174:ILE:HD12	2.15	0.45
1:E:54:TYR:CZ	1:E:131:ALA:HB2	2.51	0.45
1:E:63:ILE:O	1:E:63:ILE:HG13	2.10	0.45
1:E:94:VAL:HG23	1:E:95:HIS:N	2.32	0.45
1:A:183:ASN:OD1	1:A:184:VAL:HG23	2.17	0.45
1:D:159:VAL:O	1:D:159:VAL:HG23	2.17	0.45
1:E:20:VAL:HG22	1:E:194:VAL:HG22	1.98	0.45
1:A:62:GLU:HG3	1:A:127:VAL:HG13	1.98	0.45
1:A:39:PHE:CE1	1:A:94:VAL:HG13	2.52	0.45
1:B:10:VAL:O	1:B:12:PRO:HD3	2.16	0.45
1:D:116:ARG:HH11	1:D:116:ARG:HD3	1.64	0.45
1:E:1:GLN:NE2	1:E:1:GLN:H1	2.14	0.45
1:E:141:SER:O	1:E:143:GLY:N	2.49	0.45
1:B:186:ASN:C	1:B:186:ASN:OD1	2.59	0.45
1:E:132:SER:OG	1:E:139:GLN:NE2	2.45	0.45
1:E:54:TYR:CE1	1:E:131:ALA:HB2	2.52	0.45
1:E:186:ASN:O	1:E:188:ARG:N	2.50	0.45
1:D:1:GLN:HA	1:D:190:LEU:O	2.17	0.45
1:D:194:VAL:HG12	1:D:195:GLN:N	2.32	0.45
1:E:1:GLN:N	1:E:1:GLN:CD	2.69	0.45
1:E:62:GLU:CG	1:E:127:VAL:HG13	2.47	0.45
1:C:20:VAL:HG22	1:C:194:VAL:CG2	2.44	0.44
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.80	0.44
1:A:161:MET:HB3	1:A:185:LEU:HB2	1.98	0.44
1:B:135:LEU:HD21	1:B:159:VAL:HG11	1.98	0.44
1:C:139:GLN:HE21	1:C:143:GLY:H	1.64	0.44
1:D:26:LEU:HD12	1:D:26:LEU:HA	1.79	0.44
1:D:130:GLU:O	1:D:130:GLU:CG	2.66	0.44
1:E:137:GLN:NE2	1:E:146:PHE:HB3	2.32	0.44
1:E:181:SER:HA	1:E:182:PRO:HD3	1.76	0.44
1:A:10:VAL:O	1:A:10:VAL:HG22	2.18	0.44
1:A:57:LYS:HD3	1:A:130:GLU:CD	2.43	0.44
1:A:147:GLU:HB2	1:A:150:GLN:OE1	2.17	0.44
1:B:204:LEU:HD22	1:C:115:PRO:CB	2.48	0.44
1:E:47:ARG:HH11	1:E:47:ARG:HD3	1.60	0.44
1:B:200:THR:HG22	1:B:200:THR:O	2.17	0.43
1:D:110:TRP:CZ3	1:D:115:PRO:HB3	2.53	0.43
1:C:141:SER:O	1:C:142:PHE:C	2.59	0.43
1:A:43:LEU:O	1:A:45:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASP:O	1:D:173:THR:HG23	2.19	0.43
1:B:37:LEU:CD2	1:B:37:LEU:N	2.82	0.43
1:D:69:LYS:O	1:D:70:ASP:HB2	2.19	0.43
1:D:137:GLN:NE2	1:D:146:PHE:HB3	2.33	0.43
1:B:163:ASP:H	1:B:183:ASN:HD21	1.66	0.43
1:E:54:TYR:CD1	1:E:54:TYR:C	2.96	0.43
1:C:76:THR:HB	1:C:81:GLU:HA	2.00	0.43
1:E:56:THR:HG22	1:E:57:LYS:N	2.34	0.43
1:A:1:GLN:O	1:A:2:THR:OG1	2.33	0.43
1:D:146:PHE:CD1	1:D:146:PHE:N	2.83	0.43
1:A:77:VAL:O	1:A:77:VAL:HG22	2.19	0.43
1:A:136:GLY:O	1:A:137:GLN:CG	2.67	0.43
1:E:32:ALA:O	1:E:33:PHE:HB3	2.19	0.42
1:A:56:THR:HG22	1:A:57:LYS:N	2.33	0.42
1:E:170:GLU:O	1:E:174:ILE:HD12	2.19	0.42
1:A:3:ASP:C	1:A:3:ASP:OD1	2.61	0.42
1:E:160:ASN:HD21	1:E:187:TRP:H	1.65	0.42
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.74	0.42
1:E:176:LEU:HD12	1:E:176:LEU:HA	1.75	0.42
1:C:37:LEU:HA	1:C:158:ASN:O	2.20	0.42
1:D:62:GLU:O	1:D:78:GLY:N	2.49	0.42
1:A:169:ASP:O	1:A:173:THR:HG23	2.20	0.42
1:D:1:GLN:N	1:D:1:GLN:OE1	2.45	0.42
1:D:60:ASP:OD2	1:D:140:ASP:HA	2.18	0.42
1:A:35:VAL:HG22	1:A:161:MET:HG3	2.02	0.42
1:B:75:PHE:HB3	1:B:82:ILE:HG22	2.02	0.42
3:C:500:PC:H32	3:C:500:PC:H12	1.86	0.42
1:E:117:VAL:H	1:E:117:VAL:HG23	1.55	0.42
1:C:80:SER:HB2	1:C:122:LYS:HE3	2.02	0.41
1:E:3:ASP:HA	1:E:188:ARG:C	2.45	0.41
1:A:162:TRP:HD1	1:A:164:PHE:CE1	2.38	0.41
1:B:132:SER:HB3	1:B:139:GLN:HE22	1.84	0.41
1:E:14:GLU:CD	1:E:47:ARG:HH12	2.28	0.41
1:E:159:VAL:O	1:E:159:VAL:HG22	2.18	0.41
1:B:175:TYR:CD2	1:B:176:LEU:CD1	3.03	0.41
1:A:118:ARG:HH11	1:A:118:ARG:HD2	1.70	0.41
1:B:37:LEU:HD22	1:B:37:LEU:H	1.85	0.41
1:C:75:PHE:O	1:C:82:ILE:HG22	2.20	0.41
1:E:147:GLU:HB3	1:E:150:GLN:HB2	2.02	0.41
1:C:144:GLY:HA2	1:C:146:PHE:CZ	2.55	0.41
1:E:5:SER:O	1:E:6:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:CG	1:A:63:ILE:HG23	2.55	0.41
1:C:6:ARG:HH11	1:C:6:ARG:HD3	1.66	0.41
1:A:139:GLN:NE2	1:A:143:GLY:H	2.19	0.41
1:C:39:PHE:CD1	1:C:39:PHE:C	2.99	0.41
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.79	0.41
1:C:145:ASN:N	1:C:145:ASN:HD22	2.19	0.41
1:A:104:SER:OG	1:A:106:ILE:HG13	2.20	0.41
1:A:139:GLN:HE21	1:A:143:GLY:H	1.68	0.41
1:B:118:ARG:HH11	1:B:118:ARG:HD3	1.60	0.41
1:C:185:LEU:HD12	1:C:185:LEU:HA	1.93	0.41
1:D:47:ARG:HH12	1:D:151:SER:H	1.68	0.40
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.79	0.40
1:B:183:ASN:H	1:B:183:ASN:HD22	1.69	0.40
1:C:62:GLU:OE1	1:C:62:GLU:CA	2.56	0.40
1:D:15:SER:OG	1:D:16:ASP:N	2.54	0.40
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.72	0.40
1:B:184:VAL:HG12	1:B:185:LEU:CD1	2.49	0.40
1:C:18:SER:HA	1:C:195:GLN:O	2.21	0.40
1:E:147:GLU:HG2	1:E:150:GLN:CG	2.39	0.40
1:B:60:ASP:OD1	1:B:61:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	180 (88%)	22 (11%)	2 (1%)	12	24
1	B	204/206 (99%)	187 (92%)	15 (7%)	2 (1%)	12	24
1	C	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	12	24
1	D	204/206 (99%)	187 (92%)	15 (7%)	2 (1%)	12	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	204/206 (99%)	192 (94%)	10 (5%)	2 (1%)	12	24
All	All	1020/1030 (99%)	937 (92%)	73 (7%)	10 (1%)	12	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	142	PHE
1	C	142	PHE
1	D	117	VAL
1	E	142	PHE
1	A	87	PRO
1	B	87	PRO
1	A	142	PHE
1	D	87	PRO
1	E	87	PRO
1	C	87	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	180/180 (100%)	146 (81%)	34 (19%)	1	3
1	B	180/180 (100%)	139 (77%)	41 (23%)	1	1
1	C	180/180 (100%)	134 (74%)	46 (26%)	0	1
1	D	180/180 (100%)	146 (81%)	34 (19%)	1	3
1	E	180/180 (100%)	143 (79%)	37 (21%)	1	2
All	All	900/900 (100%)	708 (79%)	192 (21%)	1	2

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	VAL

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Mol	Chain	Res	Type
1	A	17	THR
1	A	20	VAL
1	A	22	LEU
1	A	26	LEU
1	A	30	LEU
1	A	31	LYS
1	A	43	LEU
1	A	47	ARG
1	A	56	THR
1	A	57	LYS
1	A	63	ILE
1	A	76	THR
1	A	77	VAL
1	A	89	VAL
1	A	91	VAL
1	A	102	SER
1	A	107	VAL
1	A	120	SER
1	A	121	LEU
1	A	126	THR
1	A	149	SER
1	A	151	SER
1	A	156	ILE
1	A	159	VAL
1	A	171	ILE
1	A	174	ILE
1	A	176	LEU
1	A	185	LEU
1	A	188	ARG
1	A	190	LEU
1	A	197	GLU
1	A	198	VAL
1	B	1	GLN
1	B	2	THR
1	B	5	SER
1	B	7	LYS
1	B	10	VAL
1	B	15	SER
1	B	16	ASP
1	B	21	SER
1	B	22	LEU
1	B	26	LEU

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	35	VAL
1	B	37	LEU
1	B	38	HIS
1	B	43	LEU
1	B	50	SER
1	B	51	ILE
1	B	57	LYS
1	B	63	ILE
1	B	64	LEU
1	B	74	SER
1	B	76	THR
1	B	77	VAL
1	B	83	LEU
1	B	94	VAL
1	B	99	SER
1	B	107	VAL
1	B	120	SER
1	B	130	GLU
1	B	135	LEU
1	B	149	SER
1	B	153	VAL
1	B	159	VAL
1	B	173	THR
1	B	174	ILE
1	B	176	LEU
1	B	181	SER
1	B	183	ASN
1	B	191	LYS
1	B	195	GLN
1	B	198	VAL
1	C	1	GLN
1	C	5	SER
1	C	10	VAL
1	C	22	LEU
1	C	23	LYS
1	C	26	LEU
1	C	30	LEU
1	C	38	HIS
1	C	43	LEU
1	C	45	SER
1	C	46	THR

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Mol	Chain	Res	Type
1	C	47	ARG
1	C	50	SER
1	C	56	THR
1	C	57	LYS
1	C	63	ILE
1	C	64	LEU
1	C	76	THR
1	C	77	VAL
1	C	80	SER
1	C	81	GLU
1	C	83	LEU
1	C	86	VAL
1	C	88	GLU
1	C	89	VAL
1	C	94	VAL
1	C	107	VAL
1	C	114	LYS
1	C	116	ARG
1	C	117	VAL
1	C	126	THR
1	C	134	ILE
1	C	139	GLN
1	C	147	GLU
1	C	149	SER
1	C	153	VAL
1	C	156	ILE
1	C	159	VAL
1	C	166	LEU
1	C	176	LEU
1	C	183	ASN
1	C	185	LEU
1	C	186	ASN
1	C	194	VAL
1	C	198	VAL
1	C	200	THR
1	D	1	GLN
1	D	4	MET
1	D	10	VAL
1	D	15	SER
1	D	22	LEU
1	D	26	LEU
1	D	27	THR

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Mol	Chain	Res	Type
1	D	30	LEU
1	D	38	HIS
1	D	43	LEU
1	D	50	SER
1	D	56	THR
1	D	57	LYS
1	D	60	ASP
1	D	63	ILE
1	D	64	LEU
1	D	74	SER
1	D	76	THR
1	D	77	VAL
1	D	91	VAL
1	D	98	THR
1	D	107	VAL
1	D	126	THR
1	D	135	LEU
1	D	141	SER
1	D	149	SER
1	D	155	ASP
1	D	156	ILE
1	D	159	VAL
1	D	174	ILE
1	D	181	SER
1	D	185	LEU
1	D	195	GLN
1	D	198	VAL
1	E	1	GLN
1	E	6	ARG
1	E	10	VAL
1	E	16	ASP
1	E	22	LEU
1	E	26	LEU
1	E	30	LEU
1	E	35	VAL
1	E	38	HIS
1	E	43	LEU
1	E	45	SER
1	E	56	THR
1	E	57	LYS
1	E	58	ARG
1	E	59	GLN

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Mol	Chain	Res	Type
1	E	63	ILE
1	E	68	SER
1	E	74	SER
1	E	76	THR
1	E	77	VAL
1	E	83	LEU
1	E	91	VAL
1	E	94	VAL
1	E	107	VAL
1	E	114	LYS
1	E	116	ARG
1	E	117	VAL
1	E	122	LYS
1	E	126	THR
1	E	155	ASP
1	E	159	VAL
1	E	165	VAL
1	E	171	ILE
1	E	176	LEU
1	E	181	SER
1	E	185	LEU
1	E	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	137	GLN
1	A	139	GLN
1	A	145	ASN
1	A	160	ASN
1	A	186	ASN
1	B	137	GLN
1	B	139	GLN
1	B	158	ASN
1	B	160	ASN
1	B	183	ASN
1	B	203	GLN
1	C	137	GLN
1	C	139	GLN
1	C	145	ASN
1	C	183	ASN

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Mol	Chain	Res	Type
1	C	186	ASN
1	C	203	GLN
1	D	95	HIS
1	D	137	GLN
1	D	139	GLN
1	D	145	ASN
1	D	160	ASN
1	E	1	GLN
1	E	59	GLN
1	E	137	GLN
1	E	139	GLN
1	E	145	ASN
1	E	160	ASN
1	E	195	GLN
1	E	203	GLN

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 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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
3	PC	D	500	2	10,10,10	1.61	1 (10%)	15,15,15	2.94	8 (53%)
3	PC	B	500	2	10,10,10	1.28	1 (10%)	15,15,15	2.68	6 (40%)
3	PC	A	500	2	10,10,10	1.26	2 (20%)	15,15,15	2.89	8 (53%)
3	PC	E	500	2	10,10,10	1.38	2 (20%)	15,15,15	3.74	11 (73%)
3	PC	C	500	2	10,10,10	1.49	3 (30%)	15,15,15	2.57	9 (60%)

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	PC	D	500	2	-	5/8/8/8	-
3	PC	B	500	2	-	2/8/8/8	-
3	PC	A	500	2	-	6/8/8/8	-
3	PC	E	500	2	-	7/8/8/8	-
3	PC	C	500	2	-	3/8/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	PC	C2-C1	3.35	1.61	1.51
3	B	500	PC	C2-C1	2.85	1.59	1.51
3	E	500	PC	P1-O1	2.80	1.59	1.50
3	C	500	PC	C2-C1	2.71	1.59	1.51
3	A	500	PC	C2-C1	2.49	1.58	1.51
3	A	500	PC	P1-O1	2.46	1.58	1.50
3	C	500	PC	P1-O2	-2.32	1.53	1.60
3	C	500	PC	C5-N1	-2.24	1.43	1.50
3	E	500	PC	C2-C1	2.02	1.57	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	500	PC	O2-P1-O1	6.77	124.73	106.44
3	A	500	PC	O2-P1-O1	6.27	123.39	106.44
3	B	500	PC	O4-P1-O2	6.03	122.38	106.67
3	D	500	PC	O4-P1-O2	6.01	122.34	106.67
3	E	500	PC	C5-N1-C4	-5.36	94.91	108.98
3	E	500	PC	C4-N1-C3	-4.99	95.86	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	500	PC	O4-P1-O2	4.61	118.70	106.67
3	D	500	PC	O4-P1-O3	-4.60	90.55	107.80
3	E	500	PC	C4-N1-C2	4.45	127.58	109.91
3	B	500	PC	C5-N1-C4	-4.42	97.36	108.98
3	C	500	PC	O2-P1-O1	4.31	118.08	106.44
3	A	500	PC	C5-N1-C4	-4.24	97.84	108.98
3	A	500	PC	O4-P1-O2	4.21	117.64	106.67
3	E	500	PC	C5-N1-C3	4.21	120.02	108.98
3	A	500	PC	O3-P1-O1	-4.07	95.00	110.83
3	B	500	PC	O2-P1-O1	3.99	117.22	106.44
3	D	500	PC	O2-P1-O1	3.87	116.89	106.44
3	D	500	PC	C5-N1-C3	-3.86	98.83	108.98
3	C	500	PC	C5-N1-C4	-3.83	98.92	108.98
3	E	500	PC	C1-C2-N1	3.78	127.95	115.82
3	B	500	PC	O3-P1-O1	-3.62	96.74	110.83
3	C	500	PC	C5-N1-C3	-3.56	99.63	108.98
3	E	500	PC	O3-P1-O1	-3.52	97.11	110.83
3	A	500	PC	C4-N1-C2	3.51	123.88	109.91
3	B	500	PC	C1-C2-N1	3.51	127.09	115.82
3	D	500	PC	C5-N1-C2	3.50	123.84	109.91
3	E	500	PC	P1-O2-C1	3.31	127.21	118.21
3	D	500	PC	C1-C2-N1	3.29	126.37	115.82
3	C	500	PC	O4-P1-O2	3.12	114.80	106.67
3	C	500	PC	O3-P1-O1	-3.08	98.83	110.83
3	C	500	PC	C4-N1-C2	2.94	121.60	109.91
3	E	500	PC	O4-P1-O3	-2.91	96.90	107.80
3	C	500	PC	O3-P1-O2	-2.83	99.30	106.67
3	C	500	PC	O4-P1-O3	-2.61	98.03	107.80
3	C	500	PC	O4-P1-O1	2.44	120.35	110.83
3	E	500	PC	O3-P1-O2	-2.36	100.50	106.67
3	A	500	PC	O2-C1-C2	2.32	120.83	109.65
3	D	500	PC	O3-P1-O2	2.31	112.69	106.67
3	D	500	PC	O2-C1-C2	2.28	120.64	109.65
3	A	500	PC	C1-C2-N1	2.19	122.83	115.82
3	A	500	PC	O4-P1-O1	-2.08	102.74	110.83
3	B	500	PC	C4-N1-C2	2.00	117.87	109.91

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PC	C1-O2-P1-O3

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Mol	Chain	Res	Type	Atoms
3	A	500	PC	C1-O2-P1-O4
3	B	500	PC	C1-O2-P1-O1
3	C	500	PC	C1-O2-P1-O4
3	C	500	PC	O2-C1-C2-N1
3	D	500	PC	C1-O2-P1-O4
3	D	500	PC	O2-C1-C2-N1
3	E	500	PC	C1-O2-P1-O1
3	E	500	PC	C1-O2-P1-O3
3	E	500	PC	C1-O2-P1-O4
3	E	500	PC	O2-C1-C2-N1
3	A	500	PC	C1-C2-N1-C3
3	A	500	PC	C1-C2-N1-C5
3	E	500	PC	C1-C2-N1-C5
3	A	500	PC	C1-C2-N1-C4
3	E	500	PC	C1-C2-N1-C4
3	C	500	PC	C1-O2-P1-O3
3	A	500	PC	O2-C1-C2-N1
3	B	500	PC	O2-C1-C2-N1
3	E	500	PC	C1-C2-N1-C3
3	D	500	PC	C1-O2-P1-O3
3	D	500	PC	C1-C2-N1-C3
3	D	500	PC	C1-C2-N1-C5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	500	PC	2	0
3	C	500	PC	3	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.