



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:34 am GMT

PDB ID : 1DLK  
Title : CRYSTAL STRUCTURE ANALYSIS OF DELTA-CHYMOTRYPSIN  
BOUND TO A PEPTIDYL CHLOROMETHYL KETONE INHIBITOR  
Authors : Mac Sweeney, A.; Birrane, G.; Walsh, M.A.; O'Connell, T.; Malthouse, J.P.G.  
Deposited on : 1999-12-10  
Resolution : 2.14 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

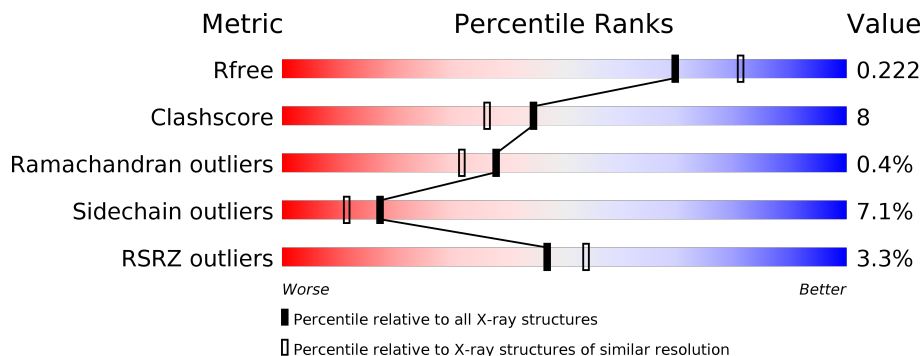
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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))
$R_{free}$	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	13	<div> <div>38%</div> <div>69%</div> <div>31%</div> </div>
1	C	13	<div> <div>62%</div> <div>15%</div> <div>15%</div> <div>8%</div> </div>
2	B	230	<div> <div>4%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
2	D	230	<div> <div>77%</div> <div>18%</div> <div>•</div> </div>
3	E	5	<div> <div>40%</div> <div>60%</div> </div>
3	F	5	<div> <div>60%</div> <div>20%</div> <div>20%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3910 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	13	Total	C	N	O	S	11	0	0
			86	56	14	15	1			
1	C	13	Total	C	N	O	S	18	0	0
			86	56	14	15	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	230	Total	C	N	O	S	17	1	0
			1700	1065	288	335	12			
2	D	230	Total	C	N	O	S	8	0	0
			1696	1062	288	335	11			

- Molecule 3 is a protein called peptidic inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	1
			30	22	3	5			
3	F	5	Total	C	N	O	0	0	1
			30	22	3	5			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

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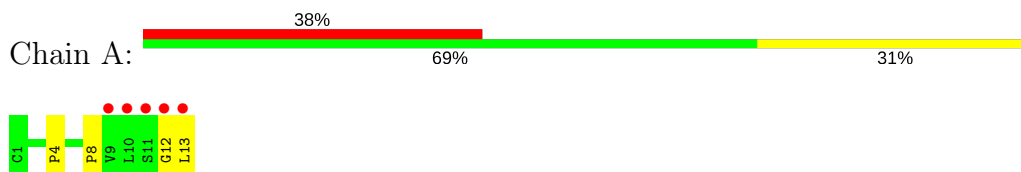
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	105	Total 105	O 105	0	0
5	C	12	Total 12	O 12	0	0
5	D	155	Total 155	O 155	0	0
5	E	1	Total 1	O 1	0	0
5	F	3	Total 3	O 3	0	0

### 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.

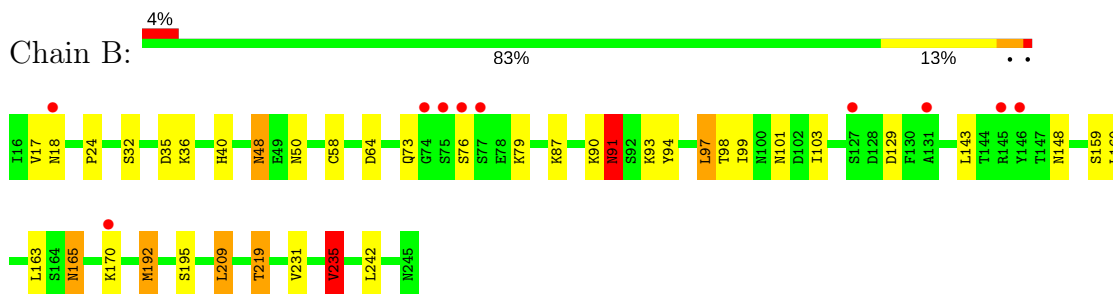
- Molecule 1: Thrombin light chain



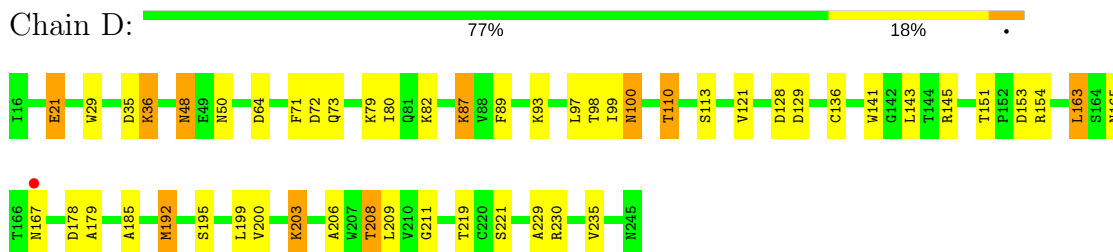
- Molecule 1: Thrombin light chain



- Molecule 2: Thrombin heavy chain



- Molecule 2: Thrombin heavy chain



- Molecule 3: peptidic inhibitor





- Molecule 3: peptidic inhibitor

Chain F:  60% 20% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.17Å 121.17Å 116.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.14 19.92 – 2.14	Depositor EDS
% Data completeness (in resolution range)	75.5 (19.90-2.14) 99.6 (19.92-2.14)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 2.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.207 , 0.245 0.194 , 0.222	Depositor DCC
$R_{free}$ test set	2428 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k 0.002 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHQ, HPH, 0QE, CL

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	1.68	2/87 (2.3%)	1.61	1/119 (0.8%)
1	C	1.77	1/87 (1.1%)	3.05	9/119 (7.6%)
2	B	0.88	5/1738 (0.3%)	1.53	24/2368 (1.0%)
2	D	0.98	2/1730 (0.1%)	1.65	27/2358 (1.1%)
3	E	6.57	3/7 (42.9%)	7.90	3/7 (42.9%)
3	F	6.23	3/7 (42.9%)	7.02	2/7 (28.6%)
All	All	1.06	16/3656 (0.4%)	1.69	66/4978 (1.3%)

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	C	0	2
2	B	1	1
2	D	1	0
3	E	0	1
All	All	2	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	LEU	CA-CB	12.56	1.82	1.53
3	E	2	GLY	N-CA	12.43	1.64	1.46
1	C	3	VAL	C-O	11.49	1.45	1.23
3	F	2	GLY	N-CA	11.32	1.63	1.46
3	E	2	GLY	CA-C	10.02	1.67	1.51
2	D	145	ARG	CD-NE	-8.99	1.31	1.46
3	F	2	GLY	CA-C	8.48	1.65	1.51
3	F	2	GLY	C-O	7.74	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	LYS	CB-CG	-7.60	1.32	1.52
2	D	79	LYS	CD-CE	-6.97	1.33	1.51
2	B	87	LYS	CG-CD	-6.19	1.31	1.52
1	A	13	LEU	CA-C	-5.90	1.37	1.52
2	B	170	LYS	CD-CE	5.86	1.65	1.51
3	E	2	GLY	C-O	5.68	1.32	1.23
2	B	192[A]	MET	CA-CB	5.60	1.66	1.53
2	B	192[B]	MET	CA-CB	5.60	1.66	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	ASP	CB-CG-OD1	15.63	132.37	118.30
1	C	3	VAL	CA-C-O	-14.54	89.57	120.10
3	E	2	GLY	CA-C-N	14.37	144.94	116.20
2	D	208	THR	CA-CB-CG2	13.18	130.85	112.40
3	F	2	GLY	CA-C-N	12.46	141.13	116.20
3	E	2	GLY	O-C-N	-12.32	102.25	123.20
3	F	2	GLY	O-C-N	-11.02	104.46	123.20
2	B	91	ASN	CA-CB-CG	10.84	137.24	113.40
1	C	3	VAL	O-C-N	-10.83	100.52	121.10
2	D	235	VAL	CG1-CB-CG2	10.80	128.18	110.90
1	C	3	VAL	C-N-CD	-10.42	97.67	120.60
2	B	93	LYS	CD-CE-NZ	-10.40	87.77	111.70
1	C	3	VAL	CA-C-N	10.13	145.47	117.10
2	B	235	VAL	CA-CB-CG2	9.29	124.83	110.90
2	B	36	LYS	CA-CB-CG	9.01	133.23	113.40
1	C	3	VAL	N-CA-C	-8.99	86.72	111.00
2	B	192[A]	MET	CA-CB-CG	-8.94	98.10	113.30
2	B	192[B]	MET	CA-CB-CG	-8.94	98.10	113.30
2	D	153	ASP	CB-CG-OD2	8.48	125.93	118.30
2	D	219	THR	CA-CB-CG2	7.91	123.47	112.40
2	D	163	LEU	CA-CB-CG	7.72	133.06	115.30
2	D	178	ASP	CB-CG-OD1	7.42	124.98	118.30
2	B	192[A]	MET	CA-C-O	-7.34	104.68	120.10
2	B	192[B]	MET	CA-C-O	-7.34	104.68	120.10
2	B	87	LYS	CB-CG-CD	7.32	130.64	111.60
1	C	3	VAL	CB-CA-C	7.26	125.20	111.40
2	D	195	SER	CB-CA-C	-7.25	96.32	110.10
2	D	154	ARG	NE-CZ-NH2	-7.04	116.78	120.30
2	D	35	ASP	CB-CG-OD1	6.88	124.50	118.30
2	D	113	SER	N-CA-CB	6.80	120.70	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	GLY	C-N-CA	6.76	136.50	122.30
2	B	24	PRO	N-CA-CB	6.75	111.41	103.30
2	D	72	ASP	CB-CG-OD2	6.70	124.33	118.30
2	D	71	PHE	CB-CG-CD1	6.66	125.46	120.80
1	C	2	GLY	C-N-CA	-6.56	105.31	121.70
2	D	82	LYS	CD-CE-NZ	6.47	126.58	111.70
2	B	219	THR	N-CA-CB	-6.38	98.18	110.30
1	C	10	LEU	CA-C-O	-6.30	106.87	120.10
2	D	208	THR	CA-CB-OG1	-6.17	96.04	109.00
2	D	219	THR	N-CA-CB	-6.16	98.60	110.30
2	D	154	ARG	CD-NE-CZ	-5.81	115.47	123.60
2	B	64	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	D	64	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	B	94	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	B	195	SER	CB-CA-C	-5.66	99.34	110.10
2	B	219	THR	CA-CB-OG1	5.62	120.81	109.00
2	B	35	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	192[A]	MET	CA-C-N	5.60	127.39	116.20
2	B	192[B]	MET	CA-C-N	5.60	127.39	116.20
1	C	10	LEU	O-C-N	5.49	131.48	122.70
2	B	87	LYS	CA-CB-CG	5.47	125.43	113.40
2	D	113	SER	CB-CA-C	-5.46	99.73	110.10
2	D	185	ALA	N-CA-CB	5.34	117.58	110.10
2	D	199	LEU	N-CA-CB	5.30	121.01	110.40
1	A	12	GLY	N-CA-C	5.30	126.35	113.10
2	D	219	THR	OG1-CB-CG2	5.26	122.10	110.00
2	B	91	ASN	CB-CG-OD1	5.26	132.12	121.60
2	B	58	CYS	CA-CB-SG	-5.21	104.62	114.00
2	D	128	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	D	21	GLU	CB-CA-C	-5.18	100.03	110.40
2	D	110	THR	CA-CB-CG2	-5.18	105.15	112.40
2	D	129	ASP	CB-CG-OD1	-5.14	113.68	118.30
2	B	235	VAL	N-CA-CB	-5.10	100.28	111.50
2	B	91	ASN	N-CA-CB	-5.10	101.42	110.60
2	B	163	LEU	CA-CB-CG	5.05	126.91	115.30
2	D	203	LYS	CB-CG-CD	5.02	124.66	111.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	219	THR	CB
2	D	219	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	91	ASN	Mainchain
1	C	3	VAL	Mainchain,Peptide
3	E	3	GLY	Mainchain

## 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	86	0	95	1	0
1	C	86	0	95	0	3
2	B	1700	0	1667	30	2
2	D	1696	0	1662	21	0
3	E	30	0	19	4	0
3	F	30	0	19	5	1
4	B	1	0	0	1	0
5	A	5	0	0	0	0
5	B	105	0	0	3	3
5	C	12	0	0	0	0
5	D	155	0	0	5	1
5	E	1	0	0	0	0
5	F	3	0	0	0	0
All	All	3910	0	3557	53	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 8.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192[B]:MET:CG	2:B:192[B]:MET:CB	1.74	1.55
2:D:48:ASN:HD22	2:D:50:ASN:H	1.30	0.79
2:B:90:LYS:NZ	4:B:400:CL:CL	2.51	0.79
2:D:208:THR:CB	5:D:402:HOH:O	2.33	0.75
2:B:91:ASN:ND2	2:B:103:ILE:HG22	2.03	0.73
2:D:48:ASN:ND2	2:D:50:ASN:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:THR:O	3:F:1:PHQ:H51	1.96	0.66
2:D:167:ASN:HB2	5:D:371:HOH:O	1.97	0.64
2:B:48:ASN:HD22	2:B:50:ASN:H	1.45	0.62
2:B:231:VAL:HG12	2:B:235:VAL:HG13	1.81	0.60
2:B:91:ASN:CG	5:B:496:HOH:O	2.39	0.60
2:B:32:SER:OG	2:B:40:HIS:HD2	1.85	0.60
2:B:48:ASN:ND2	2:B:50:ASN:H	1.99	0.59
2:D:98:THR:HA	3:F:1:PHQ:C6	2.32	0.58
2:B:91:ASN:ND2	2:B:101:ASN:HB3	2.19	0.58
2:D:98:THR:HA	3:F:1:PHQ:H61	1.84	0.57
2:B:73:GLN:NE2	5:B:475:HOH:O	2.39	0.56
2:B:98:THR:HA	3:E:1:PHQ:H51	1.87	0.55
2:B:192[B]:MET:SD	2:B:192[B]:MET:CE	2.95	0.55
2:B:98:THR:HA	3:E:1:PHQ:C5	2.37	0.54
2:D:87:LYS:HD3	2:D:89:PHE:CZ	2.43	0.54
2:D:21:GLU:HG2	5:D:359:HOH:O	2.08	0.53
2:B:192[B]:MET:SD	2:B:192[B]:MET:CB	2.93	0.53
2:B:97:LEU:O	3:E:1:PHQ:C6	2.58	0.52
2:B:91:ASN:ND2	2:B:103:ILE:CG2	2.74	0.50
2:D:143:LEU:HD12	2:D:192:MET:HE2	1.94	0.50
2:B:17:VAL:O	2:B:18:ASN:HB2	2.12	0.49
2:B:91:ASN:HD22	2:B:103:ILE:HG22	1.76	0.49
2:B:143:LEU:HD12	2:B:192[A]:MET:HB2	1.94	0.49
2:D:100:ASN:HD21	2:D:179:ALA:HB3	1.78	0.48
2:B:209:LEU:HD13	2:B:231:VAL:HG21	1.94	0.48
2:B:98:THR:HA	3:E:1:PHQ:C6	2.44	0.48
2:D:98:THR:HA	3:F:1:PHQ:C5	2.44	0.47
2:D:136:CYS:HB3	2:D:200:VAL:O	2.14	0.47
5:D:275:HOH:O	3:F:1:PHQ:H51	2.14	0.46
2:D:36:LYS:H	2:D:36:LYS:CD	2.27	0.46
1:A:4:PRO:HG2	1:A:8:PRO:HD3	1.98	0.45
2:B:48:ASN:HD22	2:B:48:ASN:C	2.19	0.44
2:D:141:TRP:O	2:D:151:THR:HB	2.18	0.44
2:D:48:ASN:HD22	2:D:48:ASN:C	2.20	0.44
2:B:48:ASN:HD22	2:B:50:ASN:N	2.15	0.42
2:B:32:SER:HG	2:B:40:HIS:HD2	1.66	0.42
2:D:206:ALA:O	2:D:208:THR:HG23	2.19	0.42
2:B:165:ASN:ND2	5:B:505:HOH:O	2.52	0.42
2:D:73:GLN:NE2	5:D:267:HOH:O	2.54	0.41
2:D:29:TRP:CG	2:D:121:VAL:HB	2.56	0.41
2:D:211:GLY:HA2	2:D:229:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192[B]:MET:HG3	2:B:192[B]:MET:CE	2.50	0.41
2:B:99:ILE:O	2:B:99:ILE:HG22	2.21	0.40
2:D:165:ASN:ND2	2:D:230:ARG:HH11	2.19	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)
1:C:3:VAL:O	5:B:456:HOH:O[8_665]	1.20	1.00
2:B:192[B]:MET:SD	5:D:356:HOH:O[3_645]	1.77	0.43
2:B:192[B]:MET:CE	3:F:2:GLY:N[3_645]	1.95	0.25
1:C:3:VAL:C	5:B:456:HOH:O[8_665]	1.98	0.22
1:C:4:PRO:N	5:B:456:HOH:O[8_665]	2.03	0.17

## 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	11/13 (85%)	11 (100%)	0	0	100	100
1	C	11/13 (85%)	9 (82%)	1 (9%)	1 (9%)	1	0
2	B	229/230 (100%)	220 (96%)	9 (4%)	0	100	100
2	D	228/230 (99%)	223 (98%)	4 (2%)	1 (0%)	38	32
3	E	1/5 (20%)	1 (100%)	0	0	100	100
3	F	1/5 (20%)	1 (100%)	0	0	100	100
All	All	481/496 (97%)	465 (97%)	14 (3%)	2 (0%)	38	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	PRO

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Mol	Chain	Res	Type
2	D	99	ILE

### 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	10/10 (100%)	10 (100%)	0	100	100
1	C	10/10 (100%)	8 (80%)	2 (20%)	1	0
2	B	189/188 (100%)	176 (93%)	13 (7%)	18	12
2	D	188/188 (100%)	175 (93%)	13 (7%)	18	12
All	All	397/396 (100%)	369 (93%)	28 (7%)	17	11

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	48	ASN
2	B	76	SER
2	B	79	LYS
2	B	97	LEU
2	B	129	ASP
2	B	148	ASN
2	B	159	SER
2	B	160	LEU
2	B	165	ASN
2	B	209	LEU
2	B	219	THR
2	B	235	VAL
2	B	242	LEU
1	C	10	LEU
1	C	13	LEU
2	D	36	LYS
2	D	48	ASN
2	D	80	ILE
2	D	87	LYS
2	D	93	LYS

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Mol	Chain	Res	Type
2	D	97	LEU
2	D	100	ASN
2	D	110	THR
2	D	163	LEU
2	D	192	MET
2	D	203	LYS
2	D	209	LEU
2	D	221	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	48	ASN
2	B	91	ASN
2	B	100	ASN
2	B	148	ASN
2	B	165	ASN
2	B	239	GLN
2	D	48	ASN
2	D	73	GLN
2	D	100	ASN
2	D	148	ASN
2	D	165	ASN
2	D	239	GLN

### 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	HPH	E	4	3,2	11,11,12	1.74	4 (36%)	11,13,15	3.16	5 (45%)
3	HPH	F	4	3,2	11,11,12	1.37	2 (18%)	11,13,15	2.82	4 (36%)

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	HPH	E	4	3,2	-	0/6/6/8	0/1/1/1
3	HPH	F	4	3,2	-	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	HPH	CB-CA	2.07	1.57	1.53
3	E	4	HPH	CZ-CE1	2.08	1.43	1.38
3	E	4	HPH	CE2-CD2	2.18	1.43	1.38
3	E	4	HPH	CE1-CD1	2.33	1.43	1.38
3	F	4	HPH	CD2-CG	2.88	1.44	1.38
3	E	4	HPH	CD2-CG	4.06	1.47	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	HPH	CB-CA-C	-7.41	97.65	112.16
3	E	4	HPH	CB-CA-C	-7.16	98.15	112.16
3	E	4	HPH	CE2-CD2-CG	-3.72	114.97	120.64
3	E	4	HPH	CB-CG-CD2	-2.36	116.14	120.91
3	E	4	HPH	CE2-CZ-CE1	-2.02	116.52	119.89
3	F	4	HPH	CE1-CD1-CG	2.15	123.91	120.64
3	F	4	HPH	CZ-CE2-CD2	2.93	124.24	120.21
3	F	4	HPH	O-C-CA	3.11	122.84	111.47
3	E	4	HPH	CZ-CE2-CD2	4.68	126.64	120.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	13/13 (100%)	1.56	5 (38%) 0 0	28, 37, 77, 80	2 (15%)
1	C	10/13 (76%)	-0.35	0 100 100	16, 30, 33, 42	0
2	B	230/230 (100%)	-0.07	10 (4%) 36 43	17, 32, 50, 78	7 (3%)
2	D	230/230 (100%)	-0.35	1 (0%) 92 94	14, 25, 42, 49	3 (1%)
3	E	2/5 (40%)	-0.26	0 100 100	26, 26, 26, 32	0
3	F	2/5 (40%)	-0.34	0 100 100	24, 24, 24, 32	0
All	All	487/496 (98%)	-0.17	16 (3%) 47 54	14, 28, 47, 80	12 (2%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	7.4
2	B	76	SER	6.7
2	B	77	SER	5.6
1	A	12	GLY	4.9
1	A	11	SER	4.4
2	B	146	TYR	3.3
1	A	9	VAL	2.9
2	B	75	SER	2.6
2	B	74	GLY	2.6
2	B	131	ALA	2.6
2	B	145	ARG	2.6
2	B	170	LYS	2.6
2	B	127	SER	2.1
2	B	18	ASN	2.1
2	D	167	ASN	2.1
1	A	10	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	HPH	F	4	11/12	0.97	0.11	-	21,22,25,25	0
3	HPH	E	4	11/12	0.96	0.10	-	25,26,29,29	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	B	400	1/1	0.80	0.42	-	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.