



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 PM UTC

PDB ID : 1NJT / pdb_00001njt
Title : COMPLEX STRUCTURE OF HCMV PROTEASE AND A PEP-
TIDOMIMETIC INHIBITOR
Authors : Khayat, R.; Batra, R.; Qian, C.; Halmos, T.; Bailey, M.; Tong, L.
Deposited on : 2003-01-02
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

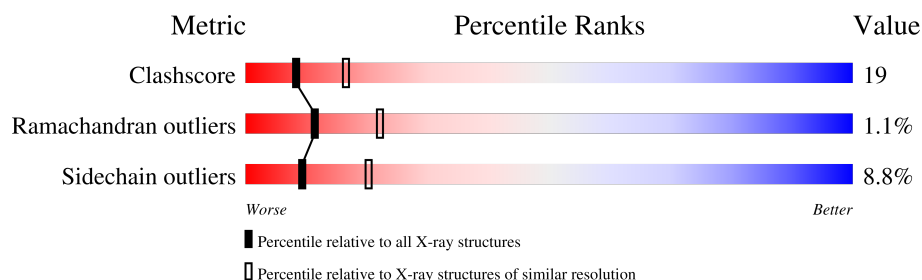
1 Overall quality at a glance

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	256	61% 22% 5% 12%
1	B	256	60% 23% 5% 11%
1	C	256	62% 21% 5% 13%
1	D	256	55% 26% 5% 13%
2	E	6	67% 17% 17%
2	F	6	67% 33%
2	G	6	67% 33%
2	H	6	67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7444 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 Capsid protein P40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1773	1109	325	332	7			
1	B	227	Total	C	N	O	S	0	0	0
			1782	1113	326	336	7			
1	C	222	Total	C	N	O	S	0	0	0
			1741	1090	317	329	5			
1	D	223	Total	C	N	O	S	0	0	0
			1745	1094	318	328	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLN	ALA	engineered mutation	UNP P16753
B	443	GLN	ALA	engineered mutation	UNP P16753
C	1143	GLN	ALA	engineered mutation	UNP P16753
D	1443	GLN	ALA	engineered mutation	UNP P16753

- Molecule 2 is a protein called Peptidomimetic Inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	F	N	O	0	0	0
			39	23	3	5	8			
2	F	6	Total	C	F	N	O	0	0	0
			39	23	3	5	8			
2	G	6	Total	C	F	N	O	0	0	0
			39	23	3	5	8			
2	H	6	Total	C	F	N	O	0	0	0
			39	23	3	5	8			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	53	Total O 53 53	0	0
4	B	83	Total O 83 83	0	0
4	C	58	Total O 58 58	0	0
4	D	45	Total O 45 45	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0

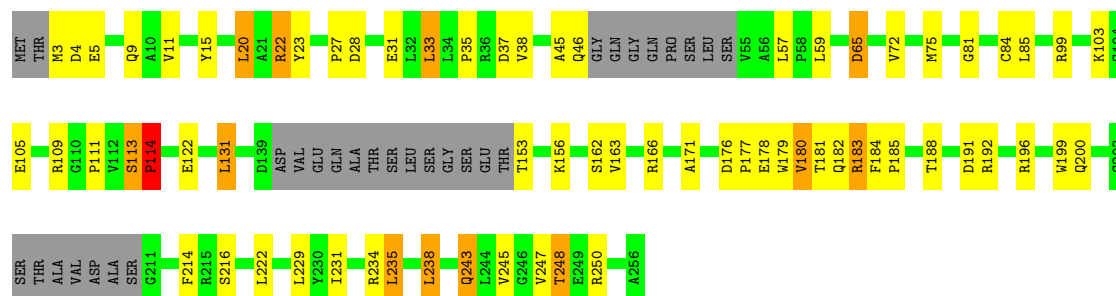
3 Residue-property plots

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.

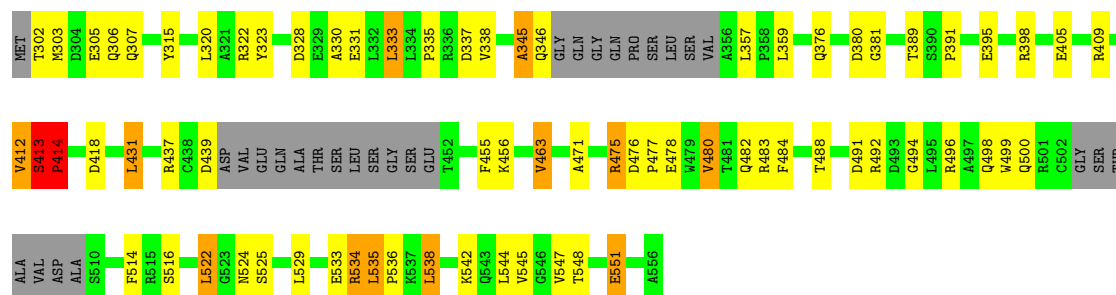
• Molecule 1: Capsid protein P40

Chain A: 



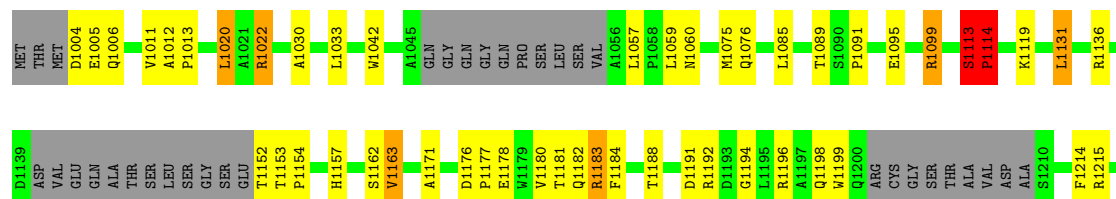
• Molecule 1: Capsid protein P40

Chain B: 



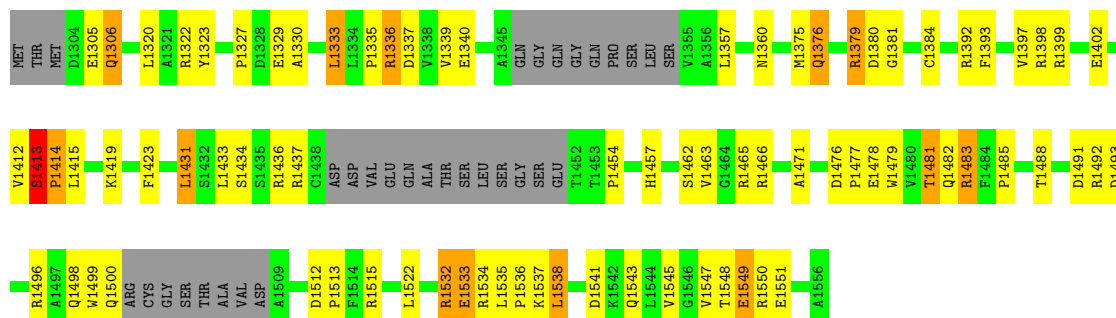
• Molecule 1: Capsid protein P40

Chain C: 

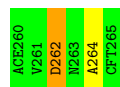




- Molecule 1: Capsid protein P40



- Molecule 2: Peptidomimetic Inhibitor



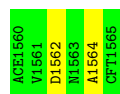
- Molecule 2: Peptidomimetic Inhibitor



- Molecule 2: Peptidomimetic Inhibitor



- Molecule 2: Peptidomimetic Inhibitor



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.07Å 213.31Å 52.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50	Depositor
% Data completeness (in resolution range)	87.6 (19.95-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7444	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ACE, DMH, CFT, DMK, 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	0.44	0/1808	0.91	2/2447 (0.1%)
1	B	0.44	0/1817	0.91	3/2460 (0.1%)
1	C	0.44	0/1776	0.90	3/2406 (0.1%)
1	D	0.43	0/1780	0.90	3/2412 (0.1%)
2	E	2.41	1/11 (9.1%)	2.07	1/13 (7.7%)
2	F	2.43	1/11 (9.1%)	2.13	1/13 (7.7%)
2	G	2.33	1/11 (9.1%)	2.23	1/13 (7.7%)
2	H	2.42	1/11 (9.1%)	2.16	1/13 (7.7%)
All	All	0.47	4/7225 (0.1%)	0.92	15/9777 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	564	ALA	C-O	7.96	1.39	1.23
2	H	1564	ALA	C-O	7.91	1.39	1.23
2	E	264	ALA	C-O	7.91	1.39	1.23
2	G	1264	ALA	C-O	7.62	1.38	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1264	ALA	CA-C-O	-7.78	107.58	120.80
2	H	1564	ALA	CA-C-O	-7.58	107.92	120.80
2	F	564	ALA	CA-C-O	-7.48	108.08	120.80
2	E	264	ALA	CA-C-O	-7.29	108.41	120.80
1	A	4	ASP	N-CA-C	-6.53	105.30	113.20
1	D	1320	LEU	N-CA-C	-5.34	106.60	113.23
1	D	1413	SER	CA-C-N	-5.33	113.18	119.84
1	D	1413	SER	C-N-CA	-5.33	113.18	119.84
1	A	20	LEU	N-CA-C	-5.30	106.65	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1113	SER	CA-C-N	-5.26	113.26	119.84
1	C	1113	SER	C-N-CA	-5.26	113.26	119.84
1	B	320	LEU	N-CA-C	-5.21	106.77	113.23
1	C	1020	LEU	N-CA-C	-5.02	107.01	113.23
1	B	413	SER	CA-C-N	-5.01	113.58	119.84
1	B	413	SER	C-N-CA	-5.01	113.58	119.84

There are no chirality outliers.

There are no planarity outliers.

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	1773	0	1743	65	0
1	B	1782	0	1750	68	0
1	C	1741	0	1708	70	0
1	D	1745	0	1718	74	0
2	E	39	0	33	1	0
2	F	39	0	33	0	0
2	G	39	0	33	0	0
2	H	39	0	33	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	53	0	0	3	0
4	B	83	0	0	5	0
4	C	58	0	0	6	0
4	D	45	0	0	6	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	7444	0	7051	274	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 19.

All (274) 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:1413:SER:HB2	1:D:1414:PRO:HD3	1.45	0.97
1:D:1436:ARG:HH11	1:D:1454:PRO:HA	1.35	0.91
1:A:113:SER:HB3	1:A:114:PRO:CD	2.03	0.88
1:D:1413:SER:CB	1:D:1414:PRO:HD3	2.03	0.88
1:B:418:ASP:OD1	1:B:475:ARG:HD2	1.72	0.88
1:C:1113:SER:HB2	1:C:1114:PRO:HD3	1.56	0.86
1:A:163:VAL:HG12	1:A:238:LEU:HD13	1.58	0.86
1:B:431:LEU:HD13	1:B:471:ALA:HB2	1.60	0.82
1:A:113:SER:HB3	1:A:114:PRO:HD3	1.61	0.81
1:D:1412:VAL:CG1	1:D:1413:SER:N	2.41	0.81
1:D:1323:TYR:CE2	1:D:1336:ARG:HD3	2.16	0.81
1:B:482:GLN:HA	1:B:492:ARG:HH21	1.46	0.80
1:C:1251:GLU:OE2	1:C:1251:GLU:HA	1.80	0.79
1:C:1131:LEU:HD13	1:C:1171:ALA:HB2	1.65	0.79
1:A:105:GLU:CD	1:A:109:ARG:HH12	1.92	0.78
1:D:1412:VAL:CG1	1:D:1413:SER:H	1.97	0.78
1:D:1431:LEU:HD13	1:D:1471:ALA:HB2	1.66	0.78
1:B:413:SER:HB3	1:B:414:PRO:CD	2.13	0.77
1:D:1551:GLU:HA	1:D:1551:GLU:OE2	1.82	0.77
1:C:1163:VAL:HG12	1:C:1238:LEU:HD13	1.65	0.77
1:B:307:GLN:HB3	4:B:20:HOH:O	1.86	0.76
1:D:1412:VAL:HG13	1:D:1413:SER:H	1.51	0.76
1:A:131:LEU:HD13	1:A:171:ALA:HB2	1.69	0.75
1:D:1436:ARG:NH1	1:D:1454:PRO:HA	2.01	0.75
1:D:1412:VAL:HG12	1:D:1413:SER:N	2.03	0.74
1:B:524:ASN:HB2	4:B:67:HOH:O	1.87	0.74
1:B:463:VAL:HG12	1:B:538:LEU:HD13	1.71	0.72
1:A:178:GLU:O	1:A:181:THR:HG22	1.91	0.70
1:D:1493:ASP:HA	1:D:1496:ARG:NH1	2.07	0.70
1:A:113:SER:CB	1:A:114:PRO:HD3	2.22	0.69
1:B:545:VAL:HG12	1:B:547:VAL:HG23	1.73	0.69
1:A:72:VAL:HG11	1:A:75:MET:HE2	1.72	0.69
1:C:1177:PRO:O	1:C:1181:THR:HG23	1.94	0.68
1:D:1419:LYS:HD2	4:D:88:HOH:O	1.92	0.68
1:D:1492:ARG:HD2	4:D:115:HOH:O	1.94	0.67
1:B:413:SER:CB	1:B:414:PRO:CD	2.74	0.66
1:C:1076:GLN:HE22	1:C:1194:GLY:HA3	1.61	0.65
1:C:1113:SER:HB2	1:C:1114:PRO:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1113:SER:CB	1:C:1114:PRO:CD	2.75	0.65
1:C:1162:SER:HB2	1:C:1234:ARG:HE	1.60	0.65
1:B:413:SER:CB	1:B:414:PRO:HD3	2.26	0.65
1:C:1004:ASP:N	1:C:1006:GLN:HE21	1.95	0.65
1:A:176:ASP:O	1:A:180:VAL:HG12	1.97	0.64
1:A:163:VAL:HG12	1:A:238:LEU:CD1	2.26	0.64
1:A:177:PRO:O	1:A:180:VAL:HG13	1.98	0.64
1:C:1022:ARG:HH11	1:C:1022:ARG:HG2	1.63	0.64
1:C:1020:LEU:HD12	1:C:1075:MET:HE3	1.80	0.63
1:D:1413:SER:HB2	1:D:1414:PRO:CD	2.25	0.63
1:B:492:ARG:HD2	4:B:32:HOH:O	1.99	0.62
1:B:492:ARG:HG3	1:B:492:ARG:HH11	1.65	0.62
1:B:542:LYS:HE3	1:B:548:THR:HG22	1.80	0.62
1:C:1113:SER:CB	1:C:1114:PRO:HD3	2.30	0.61
1:D:1413:SER:CB	1:D:1414:PRO:CD	2.75	0.61
1:C:1012:ALA:HB1	1:C:1013:PRO:HD2	1.82	0.61
1:D:1393:PHE:O	1:D:1397:VAL:HG23	2.01	0.61
1:C:1099:ARG:HH11	1:C:1099:ARG:HB3	1.65	0.61
1:C:1057:LEU:HD12	1:C:1057:LEU:H	1.65	0.61
1:C:1249:GLU:O	1:C:1250:ARG:HD2	2.00	0.61
1:C:1251:GLU:HB2	4:C:105:HOH:O	2.01	0.61
1:A:72:VAL:HG11	1:A:75:MET:CE	2.29	0.61
1:A:113:SER:CB	1:A:114:PRO:CD	2.76	0.60
1:A:196:ARG:O	1:A:200:GLN:HG3	2.02	0.60
1:B:302:THR:HB	1:B:305:GLU:HB3	1.84	0.59
1:B:413:SER:HB3	1:B:414:PRO:HD3	1.85	0.59
1:B:477:PRO:O	1:B:480:VAL:HG13	2.03	0.59
1:D:1496:ARG:O	1:D:1500:GLN:HG3	2.03	0.59
1:D:1478:GLU:O	1:D:1481:THR:HG22	2.03	0.59
1:D:1493:ASP:HA	1:D:1496:ARG:HH12	1.67	0.59
1:D:1533:GLU:HB2	1:D:1537:LYS:HE2	1.85	0.59
1:A:162:SER:HB2	1:A:234:ARG:HE	1.68	0.58
1:A:192:ARG:HD2	4:A:292:HOH:O	2.02	0.58
1:C:1182:GLN:HA	1:C:1192:ARG:HH21	1.68	0.58
1:B:456:LYS:HD2	1:B:456:LYS:N	2.16	0.58
1:B:463:VAL:HG21	1:B:534:ARG:HG3	1.86	0.58
1:C:1249:GLU:C	1:C:1250:ARG:HD2	2.29	0.57
1:B:302:THR:HB	1:B:305:GLU:CB	2.34	0.57
1:B:496:ARG:O	1:B:500:GLN:HG3	2.03	0.57
1:C:1085:LEU:HD21	1:C:1180:VAL:HG21	1.87	0.56
1:B:302:THR:O	1:B:306:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:SER:OG	1:B:414:PRO:HD3	2.05	0.56
1:C:1099:ARG:HB3	1:C:1099:ARG:NH1	2.21	0.56
1:B:389:THR:O	1:B:391:PRO:HD3	2.06	0.56
1:C:1011:VAL:HG22	1:C:1011:VAL:O	2.06	0.56
1:A:163:VAL:CG1	1:A:234:ARG:HG3	2.36	0.55
1:B:463:VAL:CG2	1:B:534:ARG:HG3	2.37	0.55
1:D:1305:GLU:HG2	1:D:1306:GLN:N	2.21	0.55
1:C:1177:PRO:O	1:C:1180:VAL:HG22	2.07	0.55
1:D:1397:VAL:HG13	1:D:1423:PHE:CD2	2.42	0.55
1:B:335:PRO:HG2	1:B:338:VAL:HG23	1.87	0.54
1:C:1057:LEU:HD12	1:C:1057:LEU:N	2.21	0.54
1:D:1336:ARG:HD2	1:D:1340:GLU:OE1	2.08	0.54
1:A:229:LEU:HD23	1:B:529:LEU:HD23	1.89	0.54
1:D:1379:ARG:HG3	1:D:1380:ASP:N	2.23	0.54
1:C:1188:THR:O	1:C:1191:ASP:HB2	2.08	0.54
1:B:337:ASP:OD2	1:B:338:VAL:N	2.41	0.53
1:B:477:PRO:HA	1:B:480:VAL:CG1	2.38	0.53
1:B:542:LYS:CE	1:B:548:THR:HG22	2.37	0.53
1:C:1163:VAL:HG12	1:C:1238:LEU:CD1	2.37	0.53
1:C:1242:LYS:HE2	1:C:1248:THR:HG22	1.91	0.53
1:D:1462:SER:HB2	1:D:1534:ARG:NH1	2.23	0.53
1:B:492:ARG:HG3	1:B:492:ARG:NH1	2.23	0.52
1:C:1030:ALA:HA	1:C:1033:LEU:CD2	2.38	0.52
1:C:1095:GLU:O	1:C:1099:ARG:HG2	2.09	0.52
1:B:488:THR:O	1:B:491:ASP:HB2	2.10	0.52
1:D:1496:ARG:HA	1:D:1499:TRP:CE2	2.44	0.52
4:A:293:HOH:O	1:D:1482:GLN:HG3	2.10	0.52
1:D:1376:GLN:NE2	1:D:1498:GLN:NE2	2.58	0.52
1:A:166:ARG:NH1	4:A:273:HOH:O	2.42	0.51
1:B:476:ASP:O	1:B:480:VAL:HG12	2.09	0.51
1:A:65:ASP:OD2	1:A:65:ASP:N	2.35	0.51
1:A:15:TYR:CZ	1:A:177:PRO:HG3	2.46	0.51
1:D:1535:LEU:HB2	1:D:1536:PRO:HD3	1.91	0.51
1:A:163:VAL:HG13	1:A:234:ARG:HG3	1.91	0.51
1:D:1335:PRO:HB2	1:D:1337:ASP:OD2	2.11	0.51
1:A:177:PRO:HA	1:A:180:VAL:CG1	2.40	0.51
1:C:1020:LEU:HD12	1:C:1075:MET:CE	2.41	0.51
1:A:178:GLU:OE2	1:A:196:ARG:NE	2.43	0.50
1:B:323:TYR:CE2	1:B:381:GLY:HA2	2.47	0.50
1:A:11:VAL:HG22	1:A:11:VAL:O	2.12	0.50
1:A:15:TYR:HD2	1:A:85:LEU:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:HG2	1:A:38:VAL:HG23	1.93	0.50
1:A:37:ASP:OD1	1:A:38:VAL:N	2.45	0.50
1:C:1194:GLY:O	1:C:1198:GLN:HG3	2.11	0.50
1:D:1413:SER:OG	1:D:1414:PRO:HD3	2.10	0.50
1:D:1376:GLN:NE2	1:D:1498:GLN:HE21	2.09	0.50
1:C:1042:TRP:HB3	1:C:1154:PRO:HG3	1.94	0.50
1:D:1488:THR:O	1:D:1491:ASP:HB2	2.13	0.49
1:A:192:ARG:HG3	1:A:192:ARG:HH11	1.76	0.49
1:C:1184:PHE:HD2	1:C:1245:VAL:CG1	2.26	0.49
1:C:1245:VAL:HG12	1:C:1245:VAL:O	2.12	0.49
1:A:31:GLU:HB2	2:E:262:DMK:OD1	2.12	0.49
1:D:1323:TYR:CE2	1:D:1381:GLY:HA2	2.47	0.49
1:D:1327:PRO:HG3	1:D:1333:LEU:HD13	1.94	0.49
1:B:315:TYR:CE1	1:B:477:PRO:HD3	2.47	0.49
1:B:534:ARG:NH1	1:B:535:LEU:HD13	2.28	0.49
1:A:188:THR:O	1:A:191:ASP:HB2	2.13	0.49
1:D:1329:GLU:OE2	1:D:1465:ARG:NH1	2.46	0.49
1:C:1030:ALA:HA	1:C:1033:LEU:HD23	1.96	0.48
1:D:1547:VAL:HG12	1:D:1547:VAL:O	2.13	0.48
1:B:551:GLU:OE1	1:B:551:GLU:HA	2.10	0.48
1:C:1057:LEU:H	1:C:1057:LEU:CD1	2.26	0.48
1:C:1233:GLU:C	1:C:1236:PRO:HD2	2.37	0.48
1:C:1196:ARG:HA	1:C:1199:TRP:CE2	2.48	0.48
1:C:1184:PHE:HB3	4:C:58:HOH:O	2.13	0.48
1:B:395:GLU:OE1	1:B:398:ARG:NH2	2.47	0.48
1:B:323:TYR:CD2	1:B:381:GLY:HA2	2.49	0.48
1:D:1330:ALA:HA	1:D:1333:LEU:CD2	2.44	0.47
1:A:182:GLN:NE2	1:A:192:ARG:HE	2.12	0.47
1:B:484:PHE:HD2	1:B:545:VAL:CG1	2.28	0.47
1:D:1463:VAL:CG2	1:D:1534:ARG:HG3	2.44	0.47
1:B:303:MET:HE2	1:B:307:GLN:NE2	2.29	0.47
1:B:496:ARG:HA	1:B:499:TRP:CE2	2.50	0.47
1:D:1433:LEU:HD12	1:D:1434:SER:H	1.80	0.47
1:D:1466:ARG:NH2	4:D:70:HOH:O	2.44	0.47
1:D:1485:PRO:HG3	1:D:1550:ARG:NH1	2.30	0.46
1:B:412:VAL:HG21	1:B:551:GLU:OE1	2.16	0.46
1:C:1192:ARG:HG3	1:C:1192:ARG:HH11	1.79	0.46
1:D:1335:PRO:O	1:D:1339:VAL:HG23	2.16	0.46
1:C:1022:ARG:HH11	1:C:1022:ARG:CG	2.27	0.46
1:B:522:LEU:O	1:B:525:SER:OG	2.30	0.46
1:A:111:PRO:HD3	1:A:122:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1180:VAL:HG23	1:C:1181:THR:N	2.30	0.46
1:D:1548:THR:HG23	1:D:1549:GLU:N	2.31	0.46
1:B:431:LEU:HD13	1:B:471:ALA:CB	2.40	0.46
1:B:478:GLU:OE2	1:B:496:ARG:NE	2.46	0.46
1:C:1060:ASN:HD21	1:C:1157:HIS:CD2	2.34	0.46
1:B:547:VAL:O	1:B:547:VAL:HG12	2.16	0.46
1:A:182:GLN:NE2	1:A:192:ARG:NE	2.63	0.45
1:A:15:TYR:CD2	1:A:85:LEU:HD11	2.51	0.45
1:A:20:LEU:HD21	1:A:84:CYS:SG	2.56	0.45
1:B:413:SER:HB3	1:B:414:PRO:HD2	1.95	0.45
1:B:482:GLN:HA	1:B:492:ARG:NH2	2.24	0.45
1:B:545:VAL:CG1	1:B:545:VAL:O	2.63	0.45
1:C:1152:THR:OG1	1:C:1153:THR:N	2.48	0.45
1:A:229:LEU:HB3	1:B:534:ARG:NH2	2.31	0.45
1:B:405:GLU:OE1	1:B:409:ARG:NH1	2.50	0.45
1:C:1182:GLN:HA	1:C:1192:ARG:NH2	2.31	0.45
1:D:1550:ARG:HG2	1:D:1550:ARG:HH11	1.81	0.45
1:A:250:ARG:HH11	1:A:250:ARG:HG2	1.82	0.45
1:B:542:LYS:C	1:B:548:THR:HG23	2.42	0.45
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.85	0.45
1:D:1412:VAL:HG12	1:D:1413:SER:OG	2.16	0.45
1:A:15:TYR:CE2	1:A:177:PRO:HG3	2.52	0.45
1:B:514:PHE:CZ	1:B:516:SER:HB3	2.52	0.45
1:D:1493:ASP:OD1	1:D:1496:ARG:NH1	2.46	0.45
1:C:1176:ASP:OD1	1:C:1177:PRO:HD2	2.17	0.45
1:A:196:ARG:HA	1:A:199:TRP:NE1	2.32	0.44
1:A:214:PHE:CZ	1:A:216:SER:HB3	2.52	0.44
1:D:1322:ARG:NH1	4:D:80:HOH:O	2.49	0.44
1:B:463:VAL:CG1	1:B:538:LEU:HD13	2.46	0.44
1:C:1214:PHE:O	1:C:1215:ARG:HD3	2.17	0.44
1:A:153:THR:O	1:A:156:LYS:HE3	2.18	0.44
1:A:247:VAL:HG12	1:A:247:VAL:O	2.18	0.44
1:C:1177:PRO:HA	1:C:1180:VAL:HG22	2.00	0.44
1:D:1533:GLU:C	1:D:1536:PRO:HD2	2.42	0.44
1:D:1360:ASN:HD21	1:D:1457:HIS:CD2	2.36	0.44
1:A:27:PRO:HG3	1:A:33:LEU:HD22	2.00	0.44
1:B:538:LEU:HD12	1:B:538:LEU:HA	1.90	0.44
1:D:1499:TRP:HH2	4:D:226:HOH:O	2.01	0.44
1:D:1533:GLU:O	1:D:1537:LYS:HG3	2.18	0.44
1:C:1020:LEU:CD1	1:C:1075:MET:HE3	2.46	0.43
4:C:82:HOH:O	1:D:1532:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:CG	1:A:33:LEU:HD22	2.48	0.43
1:C:1238:LEU:HD12	1:C:1238:LEU:HA	1.87	0.43
1:D:1376:GLN:HE21	1:D:1498:GLN:NE2	2.15	0.43
1:D:1415:LEU:HD23	1:D:1415:LEU:HA	1.86	0.43
1:A:163:VAL:HG21	1:A:231:ILE:HG21	2.01	0.43
1:B:494:GLY:O	1:B:498:GLN:HG3	2.19	0.43
1:D:1431:LEU:HD13	1:D:1471:ALA:CB	2.43	0.43
1:A:243:GLN:HE21	1:A:243:GLN:HB3	1.60	0.43
1:B:533:GLU:C	1:B:536:PRO:HD2	2.43	0.43
1:A:179:TRP:CE2	1:D:1414:PRO:HG2	2.54	0.43
1:D:1392:ARG:HG3	1:D:1512:ASP:OD2	2.18	0.43
1:A:46:GLN:HG3	1:A:153:THR:HG22	2.00	0.43
1:A:192:ARG:HG3	1:A:192:ARG:NH1	2.34	0.43
1:B:455:PHE:C	1:B:456:LYS:HD2	2.44	0.43
1:C:1131:LEU:HD13	1:C:1171:ALA:CB	2.42	0.43
1:C:1192:ARG:HG3	1:C:1192:ARG:NH1	2.34	0.43
1:C:1242:LYS:HB3	1:C:1248:THR:CG2	2.49	0.43
1:D:1376:GLN:HE21	1:D:1376:GLN:HB2	1.58	0.43
1:A:22:ARG:HA	1:A:22:ARG:HD2	1.82	0.42
1:B:476:ASP:OD2	1:B:478:GLU:HB2	2.18	0.42
1:C:1176:ASP:OD2	1:C:1178:GLU:HB2	2.18	0.42
1:C:1004:ASP:N	1:C:1006:GLN:NE2	2.65	0.42
1:B:405:GLU:CD	1:B:409:ARG:HH11	2.28	0.42
1:C:1006:GLN:CD	1:C:1006:GLN:H	2.28	0.42
1:C:1247:VAL:HG12	1:C:1247:VAL:O	2.18	0.42
1:D:1357:LEU:HD12	1:D:1357:LEU:H	1.85	0.42
1:B:330:ALA:HA	1:B:333:LEU:CD2	2.50	0.42
1:D:1463:VAL:HG22	1:D:1538:LEU:CD2	2.50	0.42
1:D:1463:VAL:HG22	1:D:1538:LEU:HD21	2.00	0.42
1:A:162:SER:O	1:A:163:VAL:HG13	2.20	0.42
1:D:1323:TYR:CD2	1:D:1381:GLY:HA2	2.54	0.42
1:D:1337:ASP:OD2	1:D:1337:ASP:N	2.52	0.42
1:A:105:GLU:CG	1:A:109:ARG:HH12	2.32	0.42
1:C:1242:LYS:HB3	1:C:1248:THR:HG23	2.02	0.42
1:A:105:GLU:HG2	1:A:109:ARG:NH1	2.35	0.41
1:C:1163:VAL:CG1	1:C:1238:LEU:HD13	2.42	0.41
1:C:1136:ARG:HG3	1:C:1136:ARG:HH11	1.83	0.41
1:D:1462:SER:C	1:D:1463:VAL:CG2	2.93	0.41
1:D:1479:TRP:O	1:D:1483:ARG:HD2	2.20	0.41
1:A:176:ASP:OD2	1:A:178:GLU:HB2	2.19	0.41
1:A:243:GLN:HA	1:A:248:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1541:ASP:O	1:D:1545:VAL:HG23	2.20	0.41
1:B:335:PRO:HG2	1:B:338:VAL:CG2	2.50	0.41
1:A:23:TYR:CE2	1:A:81:GLY:HA2	2.55	0.41
1:D:1398:ARG:NH1	1:D:1398:ARG:HG2	2.36	0.41
1:A:23:TYR:CD2	1:A:81:GLY:HA2	2.55	0.41
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.88	0.41
1:B:328:ASP:OD2	1:B:328:ASP:N	2.53	0.41
1:C:1022:ARG:CG	1:C:1022:ARG:NH1	2.82	0.41
1:C:1076:GLN:NE2	1:C:1194:GLY:HA3	2.33	0.41
1:D:1462:SER:O	1:D:1463:VAL:HG22	2.20	0.41
1:B:380:ASP:HB2	4:B:84:HOH:O	2.19	0.41
1:C:1183:ARG:N	1:C:1183:ARG:HD2	2.35	0.41
1:D:1534:ARG:HG3	1:D:1534:ARG:HH11	1.85	0.41
1:A:15:TYR:CE1	1:A:177:PRO:HG3	2.56	0.41
1:D:1437:ARG:NH1	4:D:62:HOH:O	2.54	0.41
1:A:131:LEU:HD13	1:A:171:ALA:CB	2.44	0.41
1:B:345:ALA:O	1:B:346:GLN:O	2.38	0.41
1:B:484:PHE:HD2	1:B:545:VAL:HG13	1.86	0.41
1:B:544:LEU:HD11	4:B:86:HOH:O	2.21	0.41
1:C:1119:LYS:HB2	4:C:190:HOH:O	2.20	0.41
1:A:184:PHE:HA	1:A:185:PRO:HD2	1.91	0.40
1:C:1089:THR:O	1:C:1091:PRO:HD3	2.22	0.40
1:C:1163:VAL:HG13	1:C:1238:LEU:CD2	2.51	0.40
1:C:1176:ASP:CG	4:C:165:HOH:O	2.64	0.40
1:A:179:TRP:O	1:A:183:ARG:HD2	2.22	0.40
1:C:1239:ARG:NH1	4:C:231:HOH:O	2.50	0.40
1:D:1476:ASP:HA	1:D:1477:PRO:HD2	1.97	0.40
1:D:1513:PRO:C	1:D:1515:ARG:NH1	2.80	0.40
1:A:184:PHE:HD2	1:A:245:VAL:CG1	2.35	0.40
1:B:437:ARG:HG2	1:B:439:ASP:H	1.86	0.40
1:C:1234:ARG:HH11	1:C:1234:ARG:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/256 (85%)	206 (94%)	9 (4%)	3 (1%)	9	17
1	B	219/256 (86%)	206 (94%)	10 (5%)	3 (1%)	9	17
1	C	214/256 (84%)	203 (95%)	9 (4%)	2 (1%)	14	27
1	D	215/256 (84%)	204 (95%)	9 (4%)	2 (1%)	14	27
2	E	1/6 (17%)	1 (100%)	0	0	100	100
2	F	1/6 (17%)	1 (100%)	0	0	100	100
2	G	1/6 (17%)	1 (100%)	0	0	100	100
2	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	870/1048 (83%)	823 (95%)	37 (4%)	10 (1%)	11	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ALA
1	A	113	SER
1	B	345	ALA
1	B	413	SER
1	C	1113	SER
1	D	1413	SER
1	A	114	PRO
1	B	414	PRO
1	C	1114	PRO
1	D	1414	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	191/215 (89%)	171 (90%)	20 (10%)	6	14
1	B	193/215 (90%)	175 (91%)	18 (9%)	8	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	188/215 (87%)	177 (94%)	11 (6%)	18	37
1	D	188/215 (87%)	170 (90%)	18 (10%)	8	17
2	E	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
All	All	764/864 (88%)	697 (91%)	67 (9%)	9	20

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	5	GLU
1	A	9	GLN
1	A	22	ARG
1	A	28	ASP
1	A	33	LEU
1	A	57	LEU
1	A	59	LEU
1	A	65	ASP
1	A	99	ARG
1	A	103	LYS
1	A	114	PRO
1	A	131	LEU
1	A	180	VAL
1	A	183	ARG
1	A	222	LEU
1	A	235	LEU
1	A	238	LEU
1	A	243	GLN
1	A	248	THR
1	B	322	ARG
1	B	331	GLU
1	B	333	LEU
1	B	357	LEU
1	B	359	LEU
1	B	376	GLN
1	B	412	VAL
1	B	414	PRO
1	B	431	LEU

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Mol	Chain	Res	Type
1	B	463	VAL
1	B	475	ARG
1	B	480	VAL
1	B	483	ARG
1	B	522	LEU
1	B	534	ARG
1	B	535	LEU
1	B	538	LEU
1	B	551	GLU
1	C	1005	GLU
1	C	1022	ARG
1	C	1059	LEU
1	C	1099	ARG
1	C	1114	PRO
1	C	1131	LEU
1	C	1163	VAL
1	C	1183	ARG
1	C	1222	LEU
1	C	1235	LEU
1	C	1238	LEU
1	D	1306	GLN
1	D	1333	LEU
1	D	1336	ARG
1	D	1375	MET
1	D	1376	GLN
1	D	1379	ARG
1	D	1384	CYS
1	D	1399	ARG
1	D	1402	GLU
1	D	1431	LEU
1	D	1481	THR
1	D	1483	ARG
1	D	1522	LEU
1	D	1532	ARG
1	D	1533	GLU
1	D	1538	LEU
1	D	1543	GLN
1	D	1549	GLU

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	GLN
1	A	76	GLN
1	A	182	GLN
1	A	243	GLN
1	B	306	GLN
1	B	307	GLN
1	B	309	GLN
1	B	325	GLN
1	B	362	ASN
1	B	376	GLN
1	B	482	GLN
1	B	543	GLN
1	C	1007	GLN
1	C	1025	GLN
1	C	1182	GLN
1	C	1243	GLN
1	D	1309	GLN
1	D	1325	GLN
1	D	1344	HIS
1	D	1376	GLN
1	D	1543	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
2	DMH	H	1563	2	8,9,10	0.59	0	6,11,13	0.82	0
2	DMK	F	562	2	6,9,10	1.04	0	8,13,15	1.51	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMK	H	1562	2	6,9,10	1.11	0	8,13,15	1.54	1 (12%)
2	DMH	E	263	2	8,9,10	0.68	0	6,11,13	0.52	0
2	DMH	G	1263	2	8,9,10	0.65	0	6,11,13	0.96	0
2	DMH	F	563	2	8,9,10	0.76	0	6,11,13	0.81	0
2	DMK	E	262	2	6,9,10	1.05	0	8,13,15	1.57	1 (12%)
2	DMK	G	1262	2	6,9,10	1.02	0	8,13,15	1.42	1 (12%)

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
2	DMH	H	1563	2	-	0/9/10/12	-
2	DMK	F	562	2	-	1/10/14/16	-
2	DMK	H	1562	2	-	2/10/14/16	-
2	DMH	E	263	2	-	0/9/10/12	-
2	DMH	G	1263	2	-	0/9/10/12	-
2	DMH	F	563	2	-	0/9/10/12	-
2	DMK	E	262	2	-	4/10/14/16	-
2	DMK	G	1262	2	-	0/10/14/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	262	DMK	OD1-CG1-OD2	-4.13	110.64	123.86
2	H	1562	DMK	OD1-CG1-OD2	-3.91	111.36	123.86
2	F	562	DMK	OD1-CG1-OD2	-3.69	112.05	123.86
2	G	1262	DMK	OD1-CG1-OD2	-3.57	112.42	123.86

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	262	DMK	C-CA-CB-CG2
2	E	262	DMK	C-CA-CB-CG3
2	H	1562	DMK	C-CA-CB-CG2
2	H	1562	DMK	C-CA-CB-CG3
2	E	262	DMK	CA-CB-CG1-OD1

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Mol	Chain	Res	Type	Atoms
2	E	262	DMK	CG3-CB-CG1-OD2
2	F	562	DMK	CA-CB-CG1-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	262	DMK	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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

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.