



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:11 PM UTC

PDB ID : 1IRI / pdb_00001iri
Title : Crystal structure of human autocrine motility factor complexed with an inhibitor
Authors : Tanaka, N.; Haga, A.; Uemura, H.; Akiyama, H.; Funasaka, T.; Nagase, H.; Raz, A.; Nakamura, K.T.
Deposited on : 2001-10-08
Resolution : 2.40 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

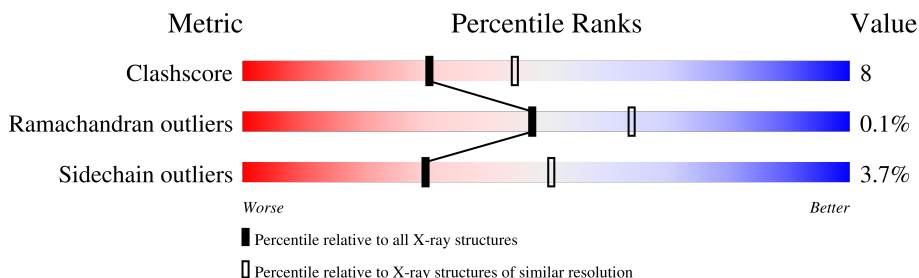
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	558	 83% 16% .
1	B	558	 79% 20% .
1	C	558	 79% 19% .
1	D	558	 78% 21% .

2 Entry composition [i](#)

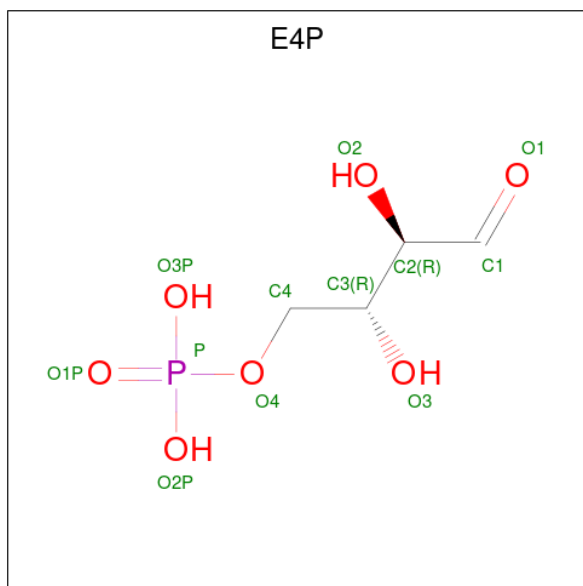
There are 3 unique types of molecules in this entry. The entry contains 18264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 autocrine motility factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4445	2832	783	811	19			
1	B	557	Total	C	N	O	S	0	0	0
			4445	2832	783	811	19			
1	C	557	Total	C	N	O	S	0	0	0
			4445	2832	783	811	19			
1	D	557	Total	C	N	O	S	0	0	0
			4445	2832	783	811	19			

- Molecule 2 is ERYTHROSE-4-PHOSPHATE (CCD ID: E4P) (formula: C₄H₉O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	1
			13	4	8	1		
2	B	1	Total	C	O	P	0	1
			13	4	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	1
			13	4	8	1		
2	D	1	Total	C	O	P	0	1
			13	4	8	1		

- Molecule 3 is water.

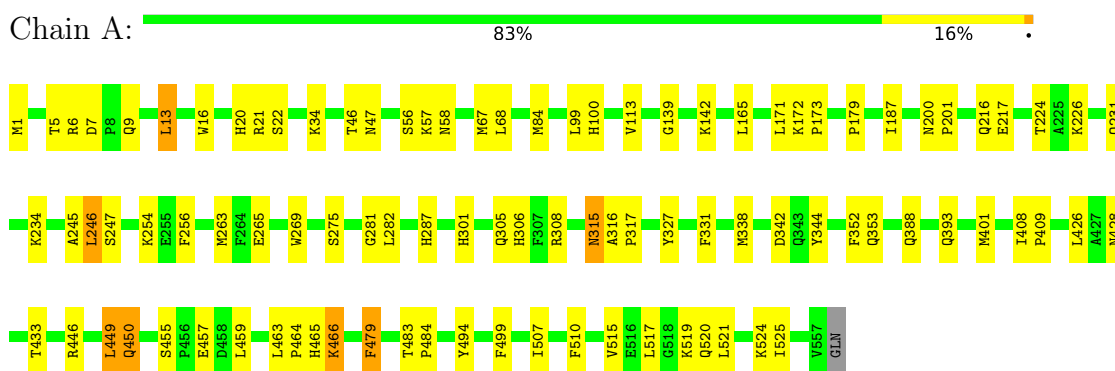
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	121	Total	O	0	0
			121	121		
3	C	109	Total	O	0	0
			109	109		
3	D	74	Total	O	0	0
			74	74		

3 Residue-property plots

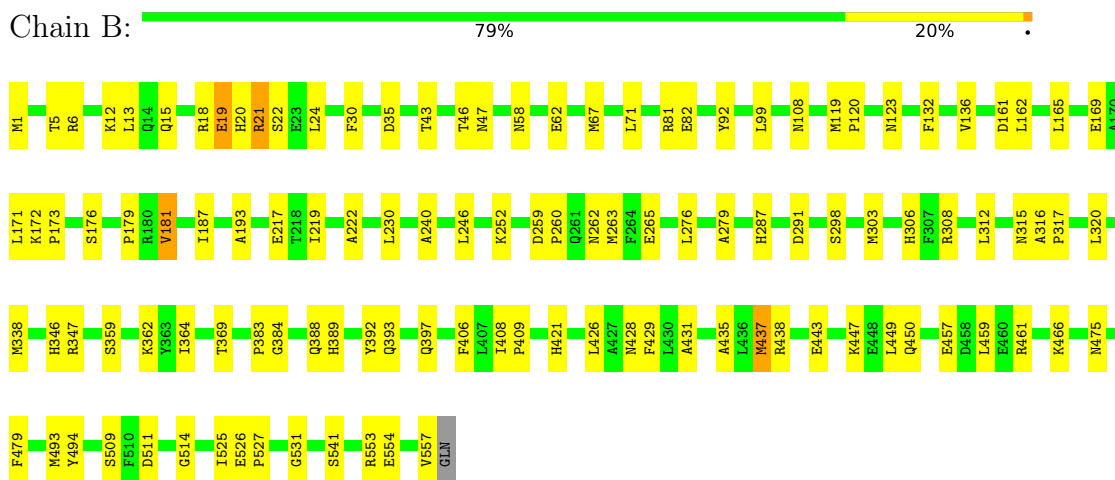
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

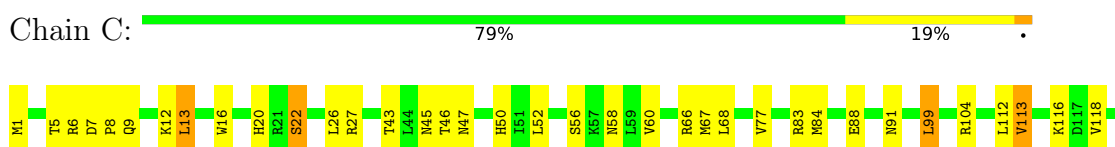
- Molecule 1: autocrine motility factor

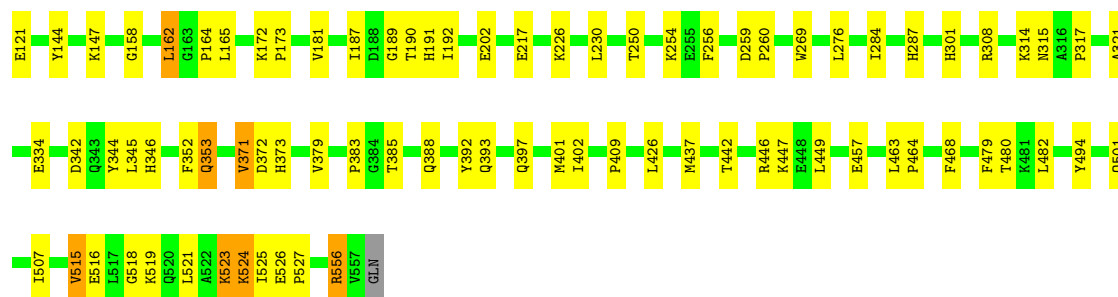


- Molecule 1: autocrine motility factor



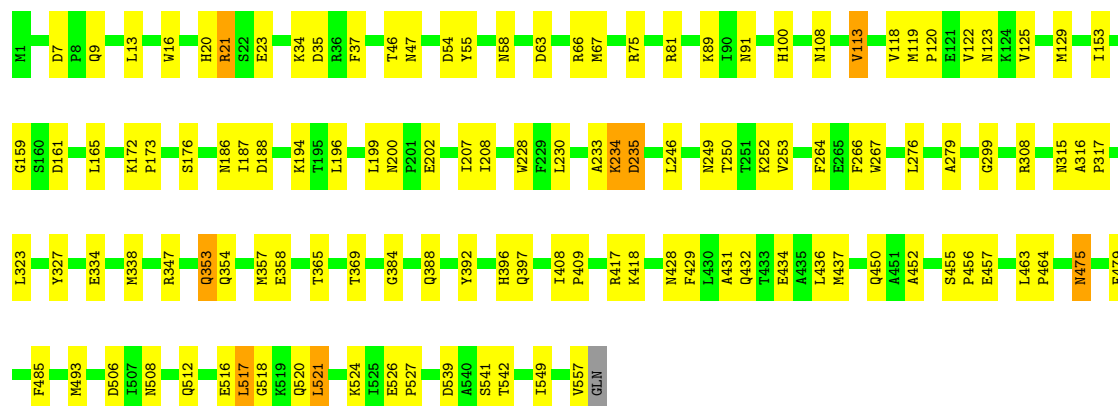
- Molecule 1: autocrine motility factor





- Molecule 1: autocrine motility factor

Chain D: 78% 21% •



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 21	Depositor
Cell constants a, b, c, α , β , γ	80.65Å 107.77Å 270.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18264	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: E4P

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	0.83	1/4553 (0.0%)	1.03	4/6164 (0.1%)
1	B	0.81	1/4553 (0.0%)	1.01	4/6164 (0.1%)
1	C	0.83	1/4553 (0.0%)	1.01	7/6164 (0.1%)
1	D	0.76	2/4553 (0.0%)	1.00	7/6164 (0.1%)
All	All	0.81	5/18212 (0.0%)	1.01	22/24656 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	MET	SD-CE	-6.68	1.62	1.79
1	A	84	MET	SD-CE	-6.43	1.63	1.79
1	C	84	MET	SD-CE	-6.14	1.64	1.79
1	B	193	ALA	CA-CB	-5.91	1.44	1.53
1	D	493	MET	SD-CE	-5.73	1.65	1.79

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	LEU	N-CA-C	6.81	118.50	111.14
1	C	353	GLN	N-CA-C	-6.78	103.89	111.28
1	B	99	LEU	N-CA-C	6.64	118.40	110.44
1	D	521	LEU	N-CA-C	6.17	118.08	111.36
1	B	92	TYR	N-CA-C	6.13	118.04	111.36
1	A	353	GLN	N-CA-C	-6.08	104.57	111.07
1	D	353	GLN	N-CA-C	-5.97	104.68	111.07
1	D	384	GLY	N-CA-C	-5.74	104.33	112.37
1	A	275	SER	N-CA-C	5.66	120.30	113.17
1	C	77	VAL	N-CA-C	5.43	116.81	110.62
1	C	308	ARG	N-CA-C	5.42	119.05	112.23
1	C	191	HIS	N-CA-C	5.37	116.82	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LEU	N-CA-C	5.36	116.80	111.07
1	A	265	GLU	N-CA-C	5.25	118.67	110.32
1	D	517	LEU	N-CA-C	-5.21	104.86	111.11
1	D	475	ASN	N-CA-C	-5.19	101.23	109.59
1	C	91	ASN	N-CA-C	-5.19	99.49	108.52
1	B	384	GLY	N-CA-C	-5.17	105.68	112.82
1	D	199	LEU	N-CA-C	5.14	117.95	109.72
1	D	397	GLN	N-CA-C	5.10	119.24	112.30
1	C	99	LEU	N-CA-C	5.10	116.56	110.44
1	A	216	GLN	N-CA-C	5.07	116.80	111.28

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	4445	0	4404	65	0
1	B	4445	0	4404	86	0
1	C	4445	0	4404	77	0
1	D	4445	0	4404	90	0
2	A	13	0	2	1	0
2	B	13	0	2	0	0
2	C	13	0	2	0	0
2	D	13	0	2	0	0
3	A	128	0	0	1	0
3	B	121	0	0	5	0
3	C	109	0	0	3	0
3	D	74	0	0	2	0
All	All	18264	0	17624	294	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 8.

All (294) 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:C:524:LYS:HB3	1:C:524:LYS:NZ	1.68	1.08
1:C:344:TYR:OH	1:D:194:LYS:NZ	1.94	1.00
1:C:524:LYS:HB3	1:C:524:LYS:HZ2	1.26	0.96
1:B:108:ASN:ND2	1:B:123:ASN:HD21	1.67	0.93
1:C:426:LEU:HD22	1:D:549:ILE:HD13	1.48	0.92
1:D:408:ILE:HG13	1:D:409:PRO:HD2	1.50	0.92
1:C:9:GLN:OE1	1:C:12:LYS:HE2	1.70	0.91
1:C:9:GLN:OE1	1:C:12:LYS:CE	2.19	0.91
1:C:9:GLN:OE1	1:C:12:LYS:NZ	2.05	0.90
1:C:144:TYR:OH	1:C:202:GLU:OE1	1.92	0.87
1:A:393:GLN:HE22	1:B:514:GLY:H	1.18	0.85
1:B:108:ASN:HD21	1:B:123:ASN:HD21	1.29	0.81
1:A:388:GLN:HE22	1:A:428:ASN:HB3	1.48	0.78
1:B:19:GLU:CD	1:B:20:HIS:CD2	2.62	0.77
1:B:263:MET:HE2	1:B:265:GLU:HG2	1.66	0.77
1:B:306:HIS:HE1	1:B:316:ALA:H	1.30	0.76
1:B:19:GLU:OE1	1:B:20:HIS:CE1	2.40	0.75
1:A:331:PHE:CD2	1:A:401:MET:HE1	2.21	0.74
1:C:393:GLN:HE22	1:C:397:GLN:HE21	1.33	0.73
1:B:19:GLU:OE1	1:B:20:HIS:CD2	2.41	0.73
1:B:291:ASP:HB2	3:B:692:HOH:O	1.89	0.72
1:D:91:ASN:ND2	1:D:508:ASN:HD21	1.88	0.72
1:A:306:HIS:HE1	1:A:316:ALA:H	1.38	0.72
1:B:82:GLU:OE1	1:B:308:ARG:NH2	2.22	0.70
1:A:224:THR:OG1	1:B:421:HIS:HE1	1.76	0.69
1:A:226:LYS:NZ	1:A:256:PHE:O	2.25	0.69
1:D:526:GLU:HB2	1:D:527:PRO:CD	2.24	0.69
1:B:388:GLN:HE22	1:B:428:ASN:HB3	1.59	0.68
1:C:46:THR:O	1:C:47:ASN:HB2	1.92	0.68
1:D:396:HIS:CD2	1:D:436:LEU:HD23	2.29	0.68
1:A:247:SER:HB3	1:A:263:MET:HE3	1.77	0.67
1:A:57:LYS:NZ	1:A:433:THR:OG1	2.27	0.67
1:D:557:VAL:HG23	1:D:557:VAL:O	1.94	0.67
1:B:19:GLU:OE1	1:B:20:HIS:NE2	2.28	0.66
1:C:524:LYS:HB3	1:C:524:LYS:HZ3	1.57	0.66
1:D:316:ALA:HB3	1:D:317:PRO:HD3	1.76	0.66
1:D:186:ASN:HD22	1:D:187:ILE:N	1.94	0.65
1:D:526:GLU:HB2	1:D:527:PRO:HD3	1.78	0.65
1:C:226:LYS:NZ	1:C:256:PHE:O	2.29	0.65
1:B:438:ARG:NE	3:B:679:HOH:O	2.05	0.64
1:C:371:VAL:HG13	1:C:373:HIS:H	1.62	0.63
1:D:108:ASN:ND2	1:D:123:ASN:HD21	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLY:O	1:B:553:ARG:NH1	2.32	0.63
1:D:20:HIS:O	1:D:21:ARG:C	2.41	0.62
1:B:108:ASN:ND2	1:B:123:ASN:ND2	2.46	0.62
1:B:393:GLN:HE22	1:B:397:GLN:HE21	1.46	0.61
1:A:393:GLN:HE22	1:B:514:GLY:N	1.95	0.61
1:D:108:ASN:HD21	1:D:123:ASN:HD21	1.47	0.61
1:D:517:LEU:O	1:D:521:LEU:HG	2.00	0.61
1:C:426:LEU:HD22	1:D:549:ILE:CD1	2.27	0.61
1:B:19:GLU:CD	1:B:20:HIS:NE2	2.59	0.61
1:B:511:ASP:OD1	3:B:635:HOH:O	2.16	0.61
1:D:7:ASP:OD1	1:D:9:GLN:N	2.34	0.61
1:A:525:ILE:HD12	1:B:431:ALA:HB2	1.82	0.60
1:A:172:LYS:N	1:A:173:PRO:CD	2.64	0.59
1:C:556:ARG:HH11	1:C:556:ARG:HG2	1.67	0.59
1:D:316:ALA:HB3	1:D:317:PRO:CD	2.32	0.59
1:B:408:ILE:HD13	1:B:426:LEU:HD23	1.84	0.59
1:C:43:THR:HG22	1:C:52:LEU:HD13	1.84	0.59
1:A:20:HIS:O	1:A:21:ARG:C	2.46	0.58
1:A:331:PHE:HD2	1:A:401:MET:HE1	1.66	0.58
1:C:353:GLN:HG3	1:C:379:VAL:O	2.02	0.58
1:D:186:ASN:HD22	1:D:187:ILE:H	1.50	0.58
1:B:46:THR:O	1:B:47:ASN:HB2	2.03	0.58
1:C:250:THR:HG22	1:C:254:LYS:HE3	1.86	0.57
1:D:46:THR:O	1:D:47:ASN:HB2	2.04	0.57
1:B:19:GLU:OE2	1:B:20:HIS:NE2	2.38	0.57
1:D:557:VAL:O	1:D:557:VAL:CG2	2.53	0.57
1:B:362:LYS:NZ	1:B:511:ASP:O	2.38	0.56
1:D:16:TRP:CG	1:D:67:MET:HE1	2.40	0.56
1:D:408:ILE:HG22	1:D:429:PHE:CZ	2.40	0.56
1:A:171:LEU:C	1:A:173:PRO:HD2	2.30	0.56
1:A:301:HIS:CE1	1:A:305:GLN:NE2	2.73	0.56
1:B:259:ASP:OD1	1:B:260:PRO:HD2	2.06	0.56
1:A:315:ASN:ND2	1:A:317:PRO:HD2	2.21	0.56
1:C:524:LYS:NZ	1:C:524:LYS:CB	2.51	0.56
1:D:75:ARG:NH2	1:D:506:ASP:HB2	2.20	0.56
1:D:408:ILE:CG1	1:D:409:PRO:HD2	2.29	0.56
1:A:139:GLY:O	1:A:142:LYS:NZ	2.39	0.55
1:B:19:GLU:OE1	1:B:20:HIS:CG	2.58	0.55
1:D:63:ASP:OD1	1:D:66:ARG:NH2	2.39	0.55
1:B:12:LYS:HD2	1:B:67:MET:SD	2.46	0.55
1:C:521:LEU:HD13	1:D:434:GLU:OE2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ILE:HG12	1:A:409:PRO:HD2	1.90	0.54
1:C:172:LYS:N	1:C:173:PRO:CD	2.70	0.54
1:C:172:LYS:HD3	1:C:287:HIS:HE1	1.72	0.54
1:A:231:GLN:O	1:A:234:LYS:HE2	2.08	0.54
1:B:457:GLU:HB2	1:B:461:ARG:NH2	2.22	0.54
1:D:165:LEU:HD23	1:D:165:LEU:C	2.33	0.53
1:D:249:ASN:O	1:D:253:VAL:HG23	2.09	0.53
1:C:371:VAL:CG1	1:C:373:HIS:H	2.21	0.53
1:C:468:PHE:CE2	1:D:517:LEU:HD22	2.44	0.53
1:B:443:GLU:OE1	1:B:447:LYS:NZ	2.36	0.52
1:D:276:LEU:C	1:D:276:LEU:HD12	2.34	0.52
1:A:408:ILE:CG1	1:A:409:PRO:HD2	2.39	0.52
2:A:601[B]:E4P:H1	1:B:389:HIS:HB3	1.91	0.52
1:C:56:SER:OG	1:D:541:SER:HB2	2.08	0.52
1:C:346:HIS:HA	1:C:383:PRO:HG3	1.91	0.52
1:D:91:ASN:C	1:D:91:ASN:HD22	2.18	0.52
1:B:108:ASN:HD21	1:B:123:ASN:ND2	2.03	0.52
1:C:259:ASP:OD1	1:C:260:PRO:HD2	2.10	0.51
1:D:396:HIS:HE1	1:D:432:GLN:OE1	1.92	0.51
1:A:315:ASN:HD22	1:A:317:PRO:HD2	1.75	0.51
1:A:224:THR:HG1	1:B:421:HIS:HE1	1.57	0.51
1:D:81:ARG:HD2	1:D:308:ARG:HA	1.92	0.51
1:B:165:LEU:C	1:B:165:LEU:HD23	2.36	0.51
1:C:342:ASP:OD2	1:C:344:TYR:HB2	2.11	0.51
1:C:165:LEU:C	1:C:165:LEU:HD23	2.35	0.51
1:C:442:THR:O	1:C:446:ARG:N	2.25	0.51
1:D:125:VAL:O	1:D:129:MET:HG3	2.11	0.51
1:D:353:GLN:O	1:D:357:MET:HB2	2.11	0.50
1:D:234:LYS:O	1:D:235:ASP:HB2	2.11	0.50
1:C:518:GLY:O	1:C:519:LYS:C	2.54	0.50
1:A:187:ILE:HB	1:A:217:GLU:HG3	1.94	0.50
1:C:371:VAL:CG1	1:C:373:HIS:O	2.59	0.50
1:C:189:GLY:O	1:C:190:THR:C	2.52	0.50
1:D:388:GLN:HE22	1:D:428:ASN:HB3	1.77	0.50
1:C:16:TRP:CG	1:C:67:MET:HE1	2.47	0.50
1:B:306:HIS:CE1	1:B:316:ALA:H	2.21	0.49
1:C:112:LEU:HA	1:C:116:LYS:O	2.12	0.49
1:A:519:LYS:O	1:A:520:GLN:C	2.53	0.49
1:B:19:GLU:HB2	3:B:693:HOH:O	2.11	0.49
1:C:385:THR:O	1:C:388:GLN:HB2	2.11	0.49
1:B:246:LEU:HD13	1:B:279:ALA:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD11	1:A:68:LEU:HD23	1.95	0.49
1:A:187:ILE:O	1:B:421:HIS:HD2	1.96	0.49
1:B:58:ASN:OD1	1:B:475:ASN:ND2	2.46	0.49
1:C:518:GLY:O	1:C:521:LEU:N	2.45	0.49
1:D:119:MET:N	1:D:120:PRO:CD	2.74	0.49
1:D:516:GLU:O	1:D:517:LEU:C	2.55	0.49
1:C:99:LEU:HB2	1:C:269:TRP:CE3	2.48	0.49
1:A:455:SER:C	1:A:457:GLU:H	2.19	0.48
1:B:181:VAL:HG22	1:B:287:HIS:CD2	2.48	0.48
1:B:132:PHE:O	1:B:136:VAL:HG23	2.12	0.48
1:A:352:PHE:CZ	1:A:494:TYR:HB2	2.48	0.48
1:A:499:PHE:HD1	1:A:510:PHE:HZ	1.62	0.48
1:B:315:ASN:OD1	1:B:317:PRO:HD2	2.14	0.48
1:A:16:TRP:CG	1:A:67:MET:HE1	2.48	0.48
1:B:406:PHE:HB3	1:B:429:PHE:CE1	2.49	0.48
1:A:165:LEU:C	1:A:165:LEU:HD23	2.39	0.48
1:A:57:LYS:HE3	1:B:541:SER:OG	2.13	0.48
1:C:83:ARG:HG2	1:C:88:GLU:CD	2.39	0.47
1:B:1:MET:HB3	1:B:6:ARG:HG3	1.96	0.47
1:D:517:LEU:HG	1:D:521:LEU:HD21	1.96	0.47
1:A:521:LEU:HB2	1:B:431:ALA:HB1	1.97	0.47
1:B:526:GLU:HB2	1:B:527:PRO:CD	2.44	0.47
1:C:26:LEU:HD13	1:C:437:MET:HG2	1.97	0.47
1:C:12:LYS:HE3	1:C:67:MET:HG2	1.97	0.47
1:B:30:PHE:CE1	1:B:437:MET:HE2	2.50	0.47
1:B:338:MET:HE3	1:B:494:TYR:CE2	2.50	0.47
1:A:99:LEU:HB2	1:A:269:TRP:CE3	2.50	0.47
1:C:162:LEU:HD12	3:C:700:HOH:O	2.14	0.47
1:A:316:ALA:HB3	1:A:317:PRO:HD3	1.97	0.46
1:B:449:LEU:HD21	1:B:466:LYS:HE3	1.97	0.46
1:D:233:ALA:O	1:D:234:LYS:C	2.58	0.46
1:D:396:HIS:CD2	1:D:436:LEU:CD2	2.97	0.46
1:B:179:PRO:O	1:B:287:HIS:HD2	1.98	0.46
1:D:323:LEU:HD13	1:D:475:ASN:HD21	1.81	0.46
1:A:171:LEU:C	1:A:173:PRO:CD	2.89	0.46
1:B:408:ILE:HG13	1:B:409:PRO:HD2	1.97	0.46
1:C:83:ARG:HG2	1:C:88:GLU:OE1	2.16	0.46
1:C:526:GLU:HB2	1:C:527:PRO:CD	2.45	0.46
1:A:449:LEU:HB3	1:A:459:LEU:HD12	1.97	0.46
1:B:169:GLU:OE2	1:B:346:HIS:NE2	2.31	0.46
1:D:200:ASN:OD1	1:D:202:GLU:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HD2	1:B:347:ARG:HA	1.71	0.46
1:C:409:PRO:HA	1:C:479:PHE:O	2.15	0.46
1:C:164:PRO:HA	1:C:284:ILE:HD11	1.98	0.46
1:A:408:ILE:CG1	1:A:409:PRO:CD	2.93	0.46
1:B:259:ASP:OD1	1:B:260:PRO:CD	2.64	0.46
1:D:365:THR:HG23	1:D:369:THR:O	2.16	0.46
1:D:539:ASP:OD2	1:D:542:THR:OG1	2.29	0.46
1:C:334:GLU:OE2	1:D:334:GLU:HG3	2.16	0.46
1:A:446:ARG:O	1:A:450:GLN:HG2	2.16	0.45
1:A:46:THR:O	1:A:47:ASN:HB2	2.17	0.45
1:A:57:LYS:CE	1:B:541:SER:OG	2.65	0.45
1:B:187:ILE:HB	1:B:217:GLU:CG	2.46	0.45
1:D:37:PHE:HB3	3:D:621:HOH:O	2.16	0.45
1:B:525:ILE:O	1:B:526:GLU:C	2.59	0.45
1:B:20:HIS:O	1:B:21:ARG:C	2.60	0.45
1:A:58:ASN:ND2	1:A:327:TYR:OH	2.41	0.45
1:C:158:GLY:HA2	3:C:700:HOH:O	2.17	0.45
1:D:409:PRO:HA	1:D:479:PHE:O	2.17	0.45
1:A:455:SER:C	1:A:457:GLU:N	2.72	0.45
1:B:19:GLU:OE2	1:B:20:HIS:CD2	2.70	0.45
1:D:388:GLN:HA	1:D:392:TYR:CG	2.52	0.45
1:A:463:LEU:HB3	1:A:464:PRO:HD3	1.98	0.45
1:C:104:ARG:O	1:C:301:HIS:HB2	2.16	0.45
1:C:315:ASN:OD1	1:C:317:PRO:HD2	2.17	0.45
1:D:113:VAL:HG13	1:D:118:VAL:HG13	1.98	0.45
1:D:408:ILE:HG13	1:D:409:PRO:CD	2.35	0.45
1:A:315:ASN:HD22	1:A:315:ASN:C	2.25	0.45
1:B:172:LYS:N	1:B:173:PRO:CD	2.80	0.45
1:A:521:LEU:HD12	1:B:435:ALA:HB2	1.99	0.44
1:B:409:PRO:HA	1:B:479:PHE:O	2.18	0.44
1:C:463:LEU:HB3	1:C:464:PRO:CD	2.47	0.44
1:D:512:GLN:N	1:D:512:GLN:CD	2.75	0.44
1:C:463:LEU:HB3	1:C:464:PRO:HD3	1.98	0.44
1:D:54:ASP:C	1:D:54:ASP:OD1	2.57	0.44
1:C:20:HIS:O	1:C:22:SER:N	2.50	0.44
1:D:75:ARG:HH21	1:D:506:ASP:HB2	1.82	0.44
1:B:81:ARG:HD2	1:B:308:ARG:HA	2.00	0.44
1:D:518:GLY:HA2	1:D:521:LEU:HD12	1.98	0.44
1:A:465:HIS:CE1	1:B:364:ILE:HG22	2.53	0.44
1:C:345:LEU:HD21	1:C:482:LEU:HD21	1.99	0.44
1:C:352:PHE:CZ	1:C:494:TYR:HB2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HD13	1:D:208:ILE:N	2.32	0.44
1:C:1:MET:HA	1:C:372:ASP:OD2	2.17	0.44
1:D:108:ASN:HD22	1:D:119:MET:HE2	1.83	0.44
1:A:465:HIS:CE1	1:B:364:ILE:CG2	3.00	0.44
1:A:466:LYS:NZ	3:A:704:HOH:O	2.47	0.44
1:C:523:LYS:HA	1:C:523:LYS:HD2	1.75	0.44
1:C:187:ILE:HB	1:C:217:GLU:HG3	1.99	0.43
1:D:187:ILE:O	1:D:187:ILE:HG13	2.16	0.43
1:D:316:ALA:CB	1:D:317:PRO:CD	2.96	0.43
1:D:485:PHE:C	1:D:485:PHE:CD2	2.96	0.43
1:A:7:ASP:OD2	1:A:9:GLN:HB2	2.18	0.43
1:A:281:GLY:O	1:A:282:LEU:C	2.61	0.43
1:C:121:GLU:HA	1:C:121:GLU:OE2	2.19	0.43
1:D:172:LYS:N	1:D:173:PRO:CD	2.81	0.43
1:B:21:ARG:HG3	1:B:22:SER:N	2.33	0.43
1:B:303:MET:HE3	1:B:493:MET:HB2	2.00	0.43
1:D:246:LEU:HD13	1:D:279:ALA:O	2.18	0.43
1:B:119:MET:N	1:B:120:PRO:CD	2.81	0.43
1:B:346:HIS:HA	1:B:383:PRO:HG3	2.00	0.43
1:B:359:SER:O	1:B:509:SER:HA	2.19	0.43
1:C:45:ASN:HB2	1:C:50:HIS:NE2	2.34	0.43
1:D:408:ILE:CG1	1:D:409:PRO:CD	2.96	0.43
1:A:342:ASP:OD2	1:A:344:TYR:HB2	2.19	0.43
1:B:388:GLN:HA	1:B:392:TYR:CG	2.53	0.43
1:C:13:LEU:HD11	1:C:68:LEU:HD23	2.01	0.43
1:D:463:LEU:HB3	1:D:464:PRO:HD3	2.00	0.43
1:A:338:MET:HE3	1:A:494:TYR:CZ	2.54	0.43
1:D:408:ILE:HG22	1:D:429:PHE:CE1	2.53	0.43
1:B:62:GLU:HG2	3:B:649:HOH:O	2.19	0.43
1:C:334:GLU:HB2	1:D:334:GLU:CD	2.43	0.42
1:C:388:GLN:HA	1:C:392:TYR:CG	2.54	0.42
1:C:480:THR:HG21	1:D:557:VAL:HG12	2.00	0.42
1:D:159:GLY:N	1:D:354:GLN:HE22	2.16	0.42
1:D:417:ARG:O	1:D:418:LYS:HB2	2.19	0.42
1:A:245:ALA:C	1:A:246:LEU:HD23	2.44	0.42
1:B:13:LEU:CD1	1:B:71:LEU:HD22	2.50	0.42
1:D:455:SER:O	1:D:456:PRO:C	2.61	0.42
1:A:200:ASN:OD1	1:A:201:PRO:HD2	2.19	0.42
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.77	0.42
1:B:459:LEU:C	1:B:459:LEU:HD23	2.44	0.42
1:D:196:LEU:HD13	1:D:228:TRP:CG	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASP:HA	1:C:8:PRO:HD3	1.86	0.42
1:C:192:ILE:HG22	3:C:640:HOH:O	2.19	0.42
1:A:409:PRO:HA	1:A:479:PHE:O	2.18	0.42
1:B:316:ALA:HB3	1:B:317:PRO:HD3	2.00	0.42
1:B:240:ALA:O	1:B:262:ASN:ND2	2.51	0.42
1:B:276:LEU:C	1:B:276:LEU:HD12	2.44	0.42
1:C:521:LEU:HB2	1:D:431:ALA:HB1	2.01	0.42
1:D:153:ILE:N	1:D:153:ILE:HD12	2.35	0.42
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.85	0.42
1:C:321:ALA:HB1	1:C:501:GLN:HG3	2.02	0.41
1:D:396:HIS:HD2	3:D:663:HOH:O	2.02	0.41
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.85	0.41
1:D:165:LEU:CD2	1:D:347:ARG:HG3	2.49	0.41
1:C:401:MET:C	1:C:402:ILE:HG13	2.44	0.41
1:B:15:GLN:HG2	1:B:18:ARG:HH22	1.85	0.41
1:D:187:ILE:O	1:D:188:ASP:C	2.63	0.41
1:C:515:VAL:CG2	1:C:516:GLU:N	2.83	0.41
1:D:207:ILE:C	1:D:208:ILE:HD13	2.46	0.41
1:A:56:SER:OG	1:B:541:SER:HB2	2.20	0.41
1:A:179:PRO:O	1:A:287:HIS:HD2	2.04	0.41
1:C:526:GLU:HB2	1:C:527:PRO:HD3	2.03	0.41
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.78	0.41
1:C:113:VAL:HG12	1:C:118:VAL:CG1	2.50	0.41
1:D:108:ASN:ND2	1:D:119:MET:HE2	2.36	0.41
1:A:1:MET:HB3	1:A:6:ARG:HE	1.86	0.41
1:A:173:PRO:HG3	1:A:344:TYR:CE1	2.56	0.41
1:A:408:ILE:HA	1:A:409:PRO:HD3	1.84	0.41
1:A:408:ILE:HD13	1:A:426:LEU:HD23	2.02	0.41
1:A:517:LEU:O	1:A:521:LEU:HG	2.20	0.41
1:B:187:ILE:HB	1:B:217:GLU:HG3	2.02	0.41
1:C:393:GLN:HB3	1:D:358:GLU:HA	2.03	0.41
1:D:108:ASN:HD22	1:D:108:ASN:HA	1.67	0.41
1:A:13:LEU:HD11	1:A:68:LEU:CD2	2.50	0.41
1:B:171:LEU:C	1:B:173:PRO:HD2	2.46	0.41
1:C:58:ASN:O	1:C:60:VAL:N	2.49	0.40
1:C:276:LEU:C	1:C:276:LEU:HD12	2.45	0.40
1:D:450:GLN:C	1:D:452:ALA:N	2.79	0.40
1:A:483:THR:HB	1:A:484:PRO:HD2	2.03	0.40
1:D:299:GLY:HA3	1:D:485:PHE:O	2.21	0.40
1:C:187:ILE:HB	1:C:217:GLU:CG	2.52	0.40
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ASN:ND2	1:D:327:TYR:OH	2.43	0.40
1:D:122:VAL:HA	1:D:267:TRP:CH2	2.56	0.40
1:B:219:ILE:O	1:B:222:ALA:HB3	2.22	0.40
1:D:55:TYR:HB2	1:D:323:LEU:HD11	2.04	0.40
1:D:234:LYS:O	1:D:235:ASP:CB	2.69	0.40
1:D:246:LEU:HA	1:D:264:PHE:O	2.22	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	555/558 (100%)	530 (96%)	25 (4%)	0	100	100
1	B	555/558 (100%)	534 (96%)	21 (4%)	0	100	100
1	C	555/558 (100%)	523 (94%)	32 (6%)	0	100	100
1	D	555/558 (100%)	525 (95%)	28 (5%)	2 (0%)	30	43
All	All	2220/2232 (100%)	2112 (95%)	106 (5%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	235	ASP
1	D	234	LYS

5.3.2 Protein sidechains [i](#)

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	476/477 (100%)	459 (96%)	17 (4%)	31	52
1	B	476/477 (100%)	460 (97%)	16 (3%)	32	54
1	C	476/477 (100%)	456 (96%)	20 (4%)	26	45
1	D	476/477 (100%)	458 (96%)	18 (4%)	29	49
All	All	1904/1908 (100%)	1833 (96%)	71 (4%)	30	51

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	13	LEU
1	A	22	SER
1	A	34	LYS
1	A	100	HIS
1	A	113	VAL
1	A	246	LEU
1	A	254	LYS
1	A	308	ARG
1	A	315	ASN
1	A	449	LEU
1	A	450	GLN
1	A	466	LYS
1	A	479	PHE
1	A	507	ILE
1	A	515	VAL
1	A	524	LYS
1	B	5	THR
1	B	19	GLU
1	B	21	ARG
1	B	24	LEU
1	B	35	ASP
1	B	43	THR
1	B	161	ASP
1	B	176	SER
1	B	181	VAL
1	B	252	LYS
1	B	298	SER
1	B	369	THR
1	B	437	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	450	GLN
1	B	554	GLU
1	B	557	VAL
1	C	5	THR
1	C	6	ARG
1	C	13	LEU
1	C	22	SER
1	C	27	ARG
1	C	66	ARG
1	C	113	VAL
1	C	147	LYS
1	C	181	VAL
1	C	314	LYS
1	C	371	VAL
1	C	447	LYS
1	C	449	LEU
1	C	457	GLU
1	C	507	ILE
1	C	515	VAL
1	C	523	LYS
1	C	524	LYS
1	C	525	ILE
1	C	556	ARG
1	D	13	LEU
1	D	21	ARG
1	D	23	GLU
1	D	34	LYS
1	D	35	ASP
1	D	89	LYS
1	D	100	HIS
1	D	113	VAL
1	D	161	ASP
1	D	176	SER
1	D	250	THR
1	D	252	LYS
1	D	266	PHE
1	D	315	ASN
1	D	437	MET
1	D	457	GLU
1	D	520	GLN
1	D	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	134	GLN
1	A	216	GLN
1	A	287	HIS
1	A	292	ASN
1	A	301	HIS
1	A	305	GLN
1	A	306	HIS
1	A	315	ASN
1	A	354	GLN
1	A	388	GLN
1	A	393	GLN
1	A	397	GLN
1	A	465	HIS
1	A	475	ASN
1	B	11	GLN
1	B	14	GLN
1	B	20	HIS
1	B	58	ASN
1	B	86	ASN
1	B	108	ASN
1	B	216	GLN
1	B	287	HIS
1	B	306	HIS
1	B	336	HIS
1	B	354	GLN
1	B	388	GLN
1	B	397	GLN
1	B	421	HIS
1	B	428	ASN
1	B	432	GLN
1	B	465	HIS
1	B	475	ASN
1	C	11	GLN
1	C	14	GLN
1	C	20	HIS
1	C	58	ASN
1	C	86	ASN
1	C	123	ASN
1	C	134	GLN
1	C	261	GLN
1	C	287	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	292	ASN
1	C	354	GLN
1	C	360	ASN
1	C	388	GLN
1	C	397	GLN
1	C	465	HIS
1	D	11	GLN
1	D	58	ASN
1	D	86	ASN
1	D	91	ASN
1	D	105	ASN
1	D	108	ASN
1	D	186	ASN
1	D	216	GLN
1	D	261	GLN
1	D	292	ASN
1	D	301	HIS
1	D	315	ASN
1	D	354	GLN
1	D	388	GLN
1	D	396	HIS
1	D	450	GLN
1	D	465	HIS
1	D	475	ASN
1	D	501	GLN
1	D	520	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands 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	E4P	B	602[A]	-	9,11,11	1.32	1 (11%)	10,15,15	1.22	1 (10%)
2	E4P	A	601[A]	-	9,11,11	1.15	1 (11%)	10,15,15	1.13	1 (10%)
2	E4P	D	604[B]	-	9,11,11	1.14	1 (11%)	10,15,15	1.41	3 (30%)
2	E4P	C	603[B]	-	9,11,11	1.37	1 (11%)	10,15,15	1.17	1 (10%)
2	E4P	B	602[B]	-	9,11,11	1.31	1 (11%)	10,15,15	1.22	1 (10%)
2	E4P	A	601[B]	-	9,11,11	1.20	1 (11%)	10,15,15	1.13	1 (10%)
2	E4P	D	604[A]	-	9,11,11	1.13	1 (11%)	10,15,15	1.41	3 (30%)
2	E4P	C	603[A]	-	9,11,11	1.36	1 (11%)	10,15,15	1.17	1 (10%)

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	E4P	B	602[A]	-	-	0/11/12/12	-
2	E4P	A	601[A]	-	-	0/11/12/12	-
2	E4P	D	604[B]	-	-	1/11/12/12	-
2	E4P	C	603[B]	-	-	0/11/12/12	-
2	E4P	B	602[B]	-	-	1/11/12/12	-
2	E4P	A	601[B]	-	-	1/11/12/12	-
2	E4P	D	604[A]	-	-	0/11/12/12	-
2	E4P	C	603[A]	-	-	0/11/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603[A]	E4P	P-O4	-3.20	1.50	1.60
2	C	603[B]	E4P	P-O4	-3.20	1.50	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602[A]	E4P	P-O4	-3.12	1.50	1.60
2	B	602[B]	E4P	P-O4	-3.12	1.50	1.60
2	D	604[A]	E4P	P-O4	-2.67	1.51	1.60
2	D	604[B]	E4P	P-O4	-2.67	1.51	1.60
2	A	601[A]	E4P	P-O4	-2.46	1.52	1.60
2	A	601[B]	E4P	P-O4	-2.46	1.52	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	E4P	C3-C2-C1	-2.39	103.83	110.53
2	A	601[B]	E4P	C3-C2-C1	-2.39	103.83	110.53
2	D	604[A]	E4P	C3-C2-C1	-2.26	104.19	110.53
2	D	604[B]	E4P	C3-C2-C1	-2.26	104.19	110.53
2	D	604[A]	E4P	O3P-P-O4	-2.17	101.02	106.67
2	D	604[B]	E4P	O3P-P-O4	-2.17	101.02	106.67
2	C	603[A]	E4P	O4-C4-C3	2.09	114.94	109.36
2	C	603[B]	E4P	O4-C4-C3	2.09	114.94	109.36
2	B	602[A]	E4P	C3-C2-C1	-2.06	104.75	110.53
2	B	602[B]	E4P	C3-C2-C1	-2.06	104.75	110.53
2	D	604[A]	E4P	O2P-P-O4	2.03	111.96	106.67
2	D	604[B]	E4P	O2P-P-O4	2.03	111.96	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[B]	E4P	O1-C1-C2-C3
2	B	602[B]	E4P	O1-C1-C2-C3
2	D	604[B]	E4P	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601[B]	E4P	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.