Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID	:	1GGU
Title	:	HUMAN FACTOR XIII WITH CALCIUM BOUND IN THE ION SITE
Authors	:	Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on	:	1998-07-22
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

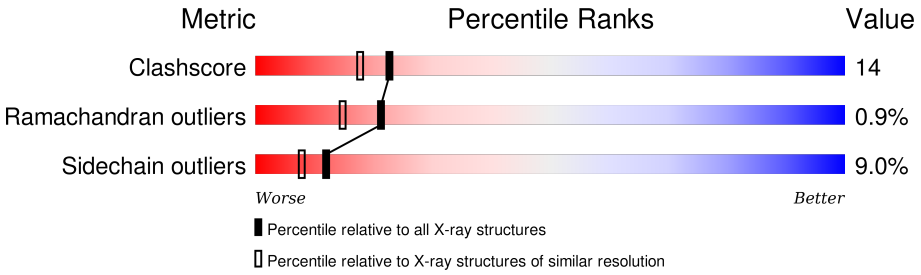
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	62% 31%
1	B	731	66% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12297 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 (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5627	3571	967	1063	26			
1	B	707	Total	C	N	O	S	0	0	0
			5667	3595	975	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLU	GLN	CONFLICT	UNP P00488
B	567	GLU	GLN	CONFLICT	UNP P00488

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total	O	0	0
			437	437		
3	B	564	Total	O	0	0
			564	564		

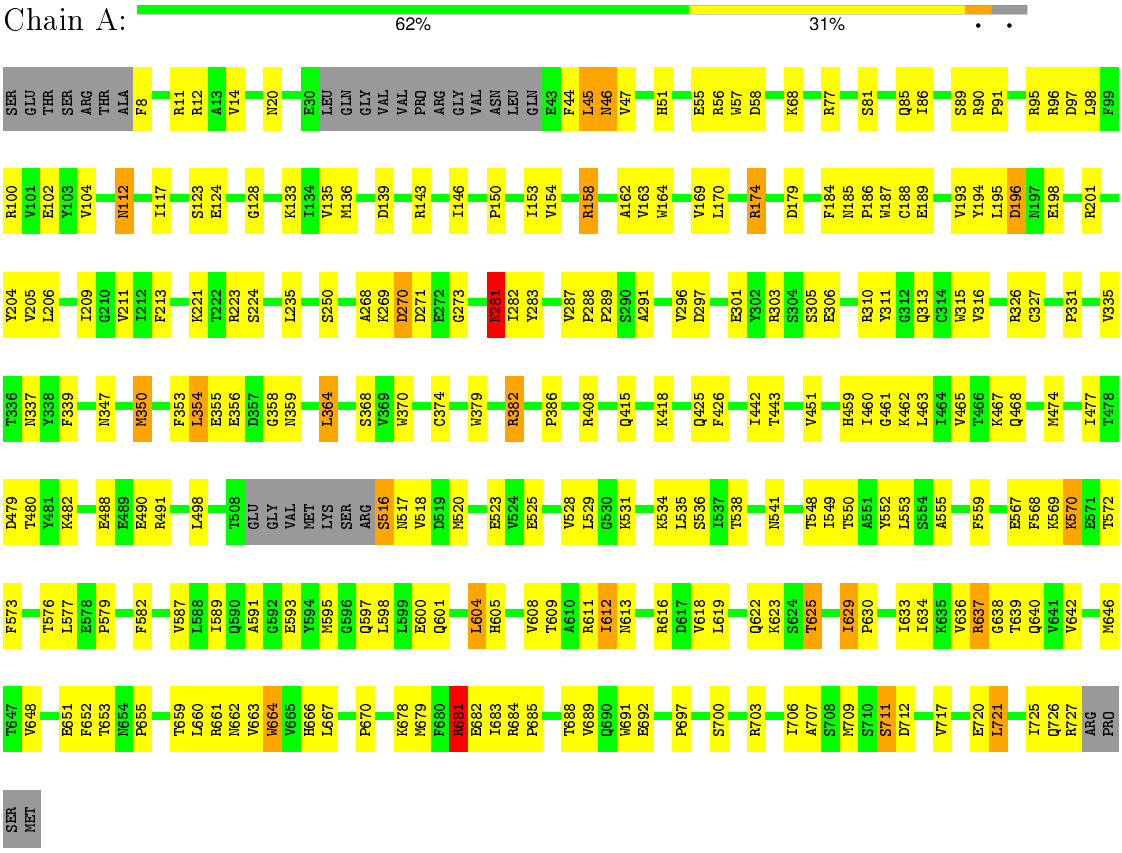
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

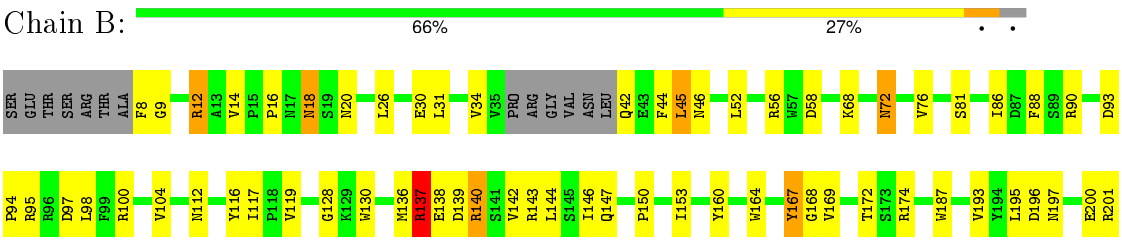
• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)

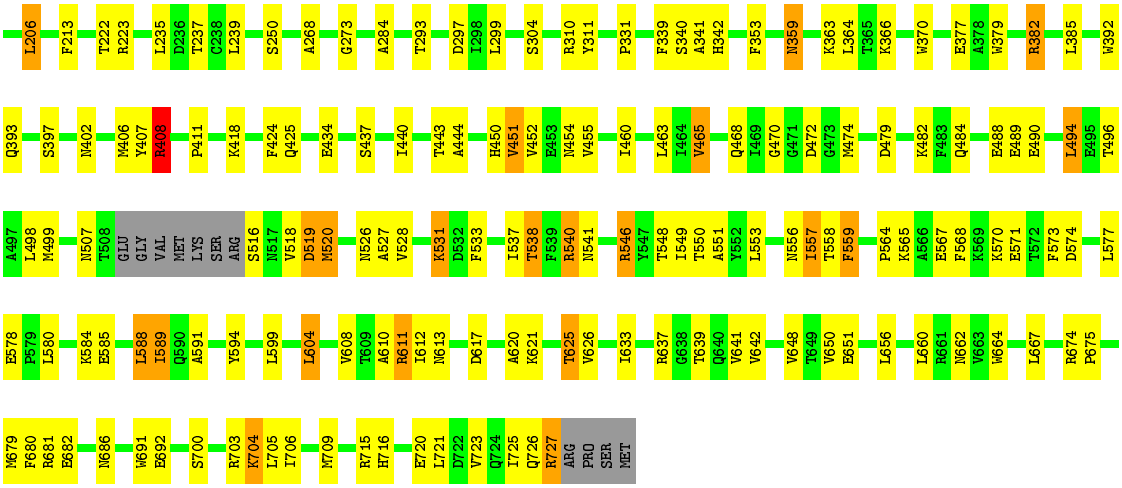
Chain A:



• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)

Chain B:




L206 F213 T222 R223 L235 D236 T237 C238 L239 S250 A268 G273 A284 T293 D297 I298 L299 S304 R310 Y311 P331 F339 S340 A341 H342 F353 N359 K363 L364 T365 K366 W370 E377 A378 W379 R382 L385 W392
Q393 S397 N402 M406 Y407 R408 P411 K418 F424 Q425 E434 S437 I440 T443 A444 H450 V451 V452 E453 N454 V455 I460 L463 I464 V465 Q468 I469 G470 G471 D472 G473 M474 D479 K482 F483 Q484 E488 E489 E490 L494 E495 T496
A497 L498 M499 N507 T508 GLU GLY VAL MET LYS SER ARG S516 N517 V518 D519 M520 N526 A527 V528 K531 D532 F533 I537 T538 F539 R540 N541 R546 Y547 T548 I549 T550 A551 Y552 L553 N556 I557 T558 F559 P564 K565 A566 E567 F568 K569 K570 E571 T572 F573 D574 L577
E578 P579 L580 K584 E585 L588 I589 Q590 A591 Y594 L599 L604 V608 T609 A610 R611 I612 N613 D617 A620 K621 T625 V626 I633 R637 G638 T639 Q640 V641 V642 V648 T649 V650 E651 L656 L660 R661 N662 V663 W664 L667 R674 P675
M679 F680 R681 E682 N686 W691 E692 S700 R703 K704 L705 I706 M709 R715 H716 E720 L721 D722 V723 Q724 I725 Q726 R727 ARG PRO SER MET

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.9 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.227 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12297	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	1/5760 (0.0%)	0.95	8/7817 (0.1%)
1	B	0.83	0/5800	0.96	9/7871 (0.1%)
All	All	0.81	1/11560 (0.0%)	0.96	17/15688 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	TRP	CB-CG	-5.13	1.41	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	LEU	N-CA-C	-7.13	91.74	111.00
1	B	9	GLY	N-CA-C	-7.06	95.45	113.10
1	A	174	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	158	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	158	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	174	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	382	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	196	ASP	N-CA-C	5.67	126.30	111.00
1	B	58	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	137	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	588	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	382	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	382	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	56	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	408	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	86	ILE	CB-CA-C	-5.13	101.34	111.60
1	A	11	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5627	0	5478	166	0
1	B	5667	0	5512	147	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	437	0	0	14	0
3	B	564	0	0	14	0
All	All	12297	0	10990	304	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 14.

All (304) 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:331:PRO:HG2	1:A:379:TRP:HB3	1.26	1.13
1:A:633:ILE:HB	1:A:651:GLU:HB3	1.51	0.89
1:B:44:PHE:O	1:B:45:LEU:HB2	1.74	0.86
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.59	0.83
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.44	0.82
1:B:31:LEU:HD22	1:B:167:TYR:O	1.82	0.79
1:A:443:THR:HB	1:A:451:VAL:HG13	1.64	0.78
1:A:567:GLU:HG2	1:A:570:LYS:HD2	1.64	0.76
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.68	0.76
1:A:518:VAL:HG12	1:A:619:LEU:HD11	1.69	0.74
1:A:44:PHE:O	1:A:45:LEU:HB2	1.86	0.73
1:B:674:ARG:HD2	1:B:675:PRO:HD2	1.71	0.73
1:A:612:ILE:HG22	1:A:613:ASN:H	1.53	0.73
1:A:136:MET:HB3	1:A:143:ARG:HB3	1.70	0.72
1:B:604:LEU:HB2	1:B:625:THR:HG22	1.69	0.72
1:A:605:HIS:CE1	1:A:622:GLN:HE21	2.08	0.71
1:B:12:ARG:HD3	3:B:6149:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:THR:HG22	1:B:613:ASN:ND2	2.07	0.70
1:A:185:ASN:ND2	1:A:188:CYS:HB2	2.06	0.70
1:B:548:THR:HG22	1:B:613:ASN:HD22	1.59	0.68
1:A:46:ASN:OD1	1:A:89:SER:HB3	1.95	0.67
1:A:666:HIS:O	1:A:707:ALA:HA	1.94	0.67
1:A:660:LEU:O	1:A:682:GLU:HA	1.95	0.67
1:A:549:ILE:HG22	1:A:550:THR:N	2.11	0.65
1:B:704:LYS:HD2	1:B:720:GLU:OE1	1.96	0.65
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.79	0.65
1:A:634:ILE:HB	1:A:721:LEU:HB2	1.79	0.65
1:B:425:GLN:HG2	3:B:6139:HOH:O	1.95	0.64
1:B:625:THR:HG21	3:B:6217:HOH:O	1.98	0.64
1:A:648:VAL:O	1:A:692:GLU:HA	1.98	0.64
1:B:100:ARG:HB2	1:B:119:VAL:O	1.98	0.64
1:A:528:VAL:HB	1:A:531:LYS:HG3	1.80	0.64
1:A:559:PHE:HD2	1:B:8:PHE:CE2	2.16	0.63
1:A:663:VAL:HA	1:A:711:SER:HA	1.80	0.63
1:A:605:HIS:HE1	1:A:622:GLN:HE21	1.46	0.63
1:A:659:THR:HG22	1:A:685:PRO:HD3	1.80	0.63
1:B:679:MET:HE1	1:B:681:ARG:HD3	1.81	0.63
1:B:359:ASN:HD21	1:B:570:LYS:HE3	1.64	0.62
1:A:518:VAL:CG1	1:A:619:LEU:HD11	2.29	0.62
1:B:546:ARG:HG3	1:B:546:ARG:NH1	2.14	0.62
1:A:569:LYS:CD	1:A:589:ILE:HD12	2.28	0.62
1:A:629:ILE:HG13	1:A:630:PRO:HD2	1.81	0.62
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.81	0.62
1:B:516:SER:N	3:B:6294:HOH:O	2.32	0.62
1:B:443:THR:HB	1:B:451:VAL:HG13	1.81	0.62
1:A:637:ARG:HG2	1:A:638:GLY:N	2.15	0.62
1:A:721:LEU:HD23	3:A:6314:HOH:O	1.99	0.62
1:A:516:SER:O	1:A:517:ASN:HB2	1.99	0.62
1:A:268:ALA:HA	1:A:273:GLY:HA3	1.82	0.61
1:A:282:ILE:HG13	1:A:283:TYR:N	2.15	0.61
1:A:569:LYS:HD3	1:A:589:ILE:HD12	1.82	0.61
1:A:623:LYS:HD2	3:A:6156:HOH:O	2.00	0.60
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.67	0.60
1:B:620:ALA:O	1:B:621:LYS:HG2	2.02	0.60
1:B:424:PHE:HB2	3:B:6348:HOH:O	2.02	0.60
1:A:162:ALA:HB3	1:A:164:TRP:CZ3	2.36	0.59
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.83	0.59
1:B:128:GLY:HA2	1:B:150:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HB	1:A:451:VAL:CG1	2.31	0.59
1:A:559:PHE:CD2	1:B:8:PHE:HE2	2.21	0.59
1:B:538:THR:HB	1:B:584:LYS:HG2	1.84	0.58
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.37	0.58
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.33	0.58
1:A:95:ARG:NH1	1:A:96:ARG:NH1	2.52	0.58
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.84	0.58
1:B:494:LEU:HD22	1:B:494:LEU:O	2.04	0.58
1:B:573:PHE:CE2	1:B:585:GLU:HG3	2.39	0.58
1:B:193:VAL:HG13	1:B:331:PRO:HD3	1.84	0.57
1:A:664:TRP:CD2	1:A:679:MET:HB2	2.39	0.57
1:A:529:LEU:HD11	1:A:598:LEU:CD1	2.34	0.57
1:B:213:PHE:CE1	1:B:474:MET:HB3	2.39	0.57
1:B:648:VAL:O	1:B:692:GLU:HA	2.04	0.57
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.85	0.57
1:A:703:ARG:HA	1:A:703:ARG:NE	2.20	0.56
1:A:418:LYS:HD2	1:A:480:THR:O	2.05	0.56
1:A:313:GLN:H	1:A:316:VAL:HB	1.69	0.56
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.16	0.56
1:A:682:GLU:CD	1:A:684:ARG:HE	2.08	0.56
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.88	0.56
1:A:95:ARG:HG2	1:A:96:ARG:HD3	1.87	0.56
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.36	0.56
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.35	0.56
1:B:553:LEU:HD23	1:B:608:VAL:CG2	2.36	0.56
1:B:549:ILE:HG22	1:B:550:THR:N	2.21	0.56
1:A:355:GLU:HG3	1:A:359:ASN:O	2.04	0.56
1:B:31:LEU:HA	1:B:168:GLY:HA3	1.88	0.56
1:A:559:PHE:HD2	1:B:8:PHE:HE2	1.54	0.56
1:A:541:ASN:ND2	1:A:579:PRO:HA	2.21	0.56
1:A:382:ARG:NH2	1:A:425:GLN:O	2.39	0.56
1:B:715:ARG:HG2	1:B:716:HIS:N	2.21	0.55
1:B:465:VAL:HG21	1:B:474:MET:SD	2.46	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:B:679:MET:HG2	1:B:680:PHE:N	2.22	0.54
1:B:553:LEU:O	1:B:570:LYS:HD2	2.08	0.54
1:B:12:ARG:HD2	1:B:16:PRO:HD3	1.90	0.54
1:A:287:VAL:HG12	1:A:288:PRO:O	2.08	0.54
1:A:55:GLU:HG3	1:A:57:TRP:CH2	2.42	0.54
1:B:139:ASP:O	1:B:140:ARG:HB2	2.06	0.54
1:A:559:PHE:CD2	1:B:8:PHE:CE2	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.43	0.54
1:A:605:HIS:CE1	1:A:622:GLN:NE2	2.77	0.53
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.89	0.53
1:B:68:LYS:HE2	1:B:206:LEU:HG	1.91	0.53
1:A:305:SER:O	1:A:306:GLU:HB2	2.06	0.53
1:A:95:ARG:O	1:A:96:ARG:HD2	2.08	0.53
1:A:559:PHE:HB2	1:B:8:PHE:HE2	1.72	0.53
1:B:520:MET:HE2	1:B:621:LYS:HG3	1.90	0.53
1:B:537:ILE:HD12	1:B:573:PHE:CZ	2.44	0.53
1:A:541:ASN:HB2	1:A:577:LEU:HD13	1.90	0.53
1:A:459:HIS:HA	1:A:462:LYS:HE3	1.90	0.53
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.44	0.53
1:A:335:VAL:O	1:A:374:CYS:HA	2.09	0.52
1:A:281:ASN:HD21	1:A:600:GLU:HG2	1.74	0.52
1:B:664:TRP:O	1:B:709:MET:HA	2.09	0.52
1:A:653:THR:O	1:A:655:PRO:HD3	2.10	0.52
1:B:650:VAL:HG22	1:B:691:TRP:HB3	1.90	0.52
1:B:72:ASN:HD22	1:B:72:ASN:H	1.55	0.52
1:B:549:ILE:HG12	1:B:612:ILE:HG12	1.92	0.52
1:A:425:GLN:HB2	1:A:426:PHE:CD2	2.45	0.52
1:B:541:ASN:O	1:B:580:LEU:HA	2.09	0.51
1:B:284:ALA:HB3	3:B:6521:HOH:O	2.10	0.51
1:B:528:VAL:HB	1:B:531:LYS:HG3	1.93	0.51
1:A:720:GLU:HG3	3:A:6312:HOH:O	2.09	0.51
1:A:663:VAL:HG13	1:A:709:MET:SD	2.51	0.51
1:B:553:LEU:O	1:B:570:LYS:HA	2.11	0.51
1:B:140:ARG:NH1	3:B:6420:HOH:O	2.42	0.51
1:A:331:PRO:HG2	1:A:379:TRP:CB	2.19	0.51
1:A:612:ILE:HG22	1:A:613:ASN:N	2.24	0.51
1:B:558:THR:HG22	1:B:564:PRO:HA	1.92	0.51
1:A:538:THR:CG2	1:A:582:PHE:CZ	2.93	0.51
1:B:662:ASN:N	1:B:662:ASN:HD22	2.07	0.51
1:B:533:PHE:CE1	1:B:589:ILE:HG13	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:CZ	2.41	0.51
1:A:12:ARG:HH22	1:B:406:MET:CE	2.24	0.51
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.46	0.51
1:A:189:GLU:HA	1:A:194:TYR:CD1	2.46	0.50
1:A:353:PHE:CD2	1:A:364:LEU:HB3	2.46	0.50
1:A:356:GLU:O	1:A:611:ARG:NE	2.44	0.50
1:A:189:GLU:HA	1:A:194:TYR:CG	2.46	0.50
1:B:56:ARG:HD3	3:B:6081:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG12	3:A:6244:HOH:O	2.11	0.50
1:B:452:VAL:O	1:B:452:VAL:HG13	2.11	0.50
1:A:112:ASN:HB2	3:A:6073:HOH:O	2.11	0.50
1:A:296:VAL:HG21	3:A:6212:HOH:O	2.12	0.49
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.94	0.49
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.45	0.49
1:B:86:ILE:HD12	1:B:144:LEU:HD11	1.93	0.49
1:A:683:ILE:HG12	1:A:689:VAL:HG11	1.94	0.49
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.42	0.49
1:A:516:SER:N	3:A:6284:HOH:O	2.45	0.49
1:A:209:ILE:HG12	1:A:670:PRO:CG	2.42	0.49
1:A:44:PHE:O	1:A:45:LEU:CB	2.58	0.49
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.94	0.49
1:B:526:ASN:HB3	3:B:6198:HOH:O	2.13	0.49
1:B:93:ASP:O	1:B:95:ARG:N	2.46	0.49
1:A:552:TYR:O	1:A:608:VAL:HA	2.13	0.49
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.94	0.49
1:B:716:HIS:CE1	3:B:6556:HOH:O	2.66	0.48
1:A:568:PHE:HB2	1:A:593:GLU:O	2.13	0.48
1:B:454:ASN:ND2	3:B:6060:HOH:O	2.46	0.48
1:A:573:PHE:HE1	3:A:6168:HOH:O	1.96	0.48
1:B:26:LEU:HD12	1:B:160:TYR:CE2	2.48	0.48
1:A:337:ASN:OD1	1:A:461:GLY:HA2	2.13	0.48
1:A:196:ASP:HB2	3:A:6125:HOH:O	2.13	0.48
1:A:102:GLU:HA	1:A:117:ILE:O	2.13	0.48
1:B:137:ARG:HG2	1:B:142:VAL:HG12	1.95	0.48
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.78	0.48
1:A:313:GLN:OE1	1:A:315:TRP:CH2	2.66	0.48
1:B:551:ALA:HA	1:B:610:ALA:HA	1.96	0.48
1:A:68:LYS:HG3	3:A:6049:HOH:O	2.13	0.48
1:B:490:GLU:O	1:B:490:GLU:HG2	2.14	0.48
1:B:397:SER:HA	1:B:408:ARG:HB3	1.94	0.48
1:A:535:LEU:HD23	1:A:536:SER:N	2.29	0.48
1:A:634:ILE:HD12	1:A:720:GLU:HA	1.96	0.48
1:A:297:ASP:OD1	1:A:297:ASP:N	2.46	0.47
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.49	0.47
1:A:640:GLN:HG2	1:A:646:MET:SD	2.54	0.47
1:B:418:LYS:NZ	1:B:479:ASP:O	2.39	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.13	0.47
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.48	0.47
1:A:339:PHE:HA	1:A:370:TRP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB3	1:A:706:ILE:HD11	1.96	0.47
1:B:81:SER:HA	1:B:146:ILE:O	2.14	0.47
1:A:652:PHE:O	1:A:688:THR:HA	2.15	0.47
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.79	0.47
1:B:268:ALA:HA	1:B:273:GLY:HA3	1.96	0.47
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.97	0.46
1:B:402:ASN:HD21	1:B:407:TYR:HB2	1.80	0.46
1:B:553:LEU:HD23	1:B:608:VAL:HG22	1.96	0.46
1:B:703:ARG:HB2	1:B:723:VAL:HG23	1.97	0.46
1:A:358:GLY:O	1:A:609:THR:HB	2.15	0.46
1:B:128:GLY:HA2	1:B:150:PRO:CD	2.45	0.46
1:A:683:ILE:HD11	1:A:689:VAL:HG21	1.98	0.46
1:A:163:VAL:N	1:A:170:LEU:O	2.42	0.46
1:A:354:LEU:O	1:A:443:THR:HA	2.15	0.46
1:B:705:LEU:O	1:B:720:GLU:HA	2.15	0.46
1:A:538:THR:HG21	1:A:582:PHE:CZ	2.49	0.46
1:A:153:ILE:HD11	1:A:250:SER:HA	1.98	0.46
1:B:339:PHE:HA	1:B:370:TRP:O	2.16	0.46
1:B:706:ILE:HG21	3:B:6430:HOH:O	2.16	0.46
1:A:8:PHE:CE2	1:B:559:PHE:CD1	3.04	0.46
1:B:559:PHE:HD1	1:B:599:LEU:HD13	1.79	0.46
1:A:128:GLY:HA2	1:A:150:PRO:HD3	1.98	0.46
1:B:660:LEU:O	1:B:682:GLU:HA	2.15	0.46
1:A:667:LEU:HA	1:A:706:ILE:O	2.16	0.45
1:A:418:LYS:HE3	1:A:479:ASP:O	2.16	0.45
1:B:541:ASN:HB2	1:B:577:LEU:HD13	1.98	0.45
1:B:715:ARG:HG2	1:B:716:HIS:H	1.81	0.45
1:B:679:MET:HE2	1:B:679:MET:HB3	1.91	0.45
1:A:296:VAL:HB	3:A:6019:HOH:O	2.15	0.45
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.52	0.45
1:B:297:ASP:N	1:B:297:ASP:OD1	2.49	0.45
1:A:162:ALA:HB3	1:A:164:TRP:HZ3	1.79	0.45
1:B:197:ASN:ND2	1:B:200:GLU:OE1	2.42	0.45
1:B:18:ASN:HD22	1:B:18:ASN:C	2.21	0.45
1:A:726:GLN:O	1:A:727:ARG:HB3	2.17	0.45
1:B:496:THR:O	1:B:499:MET:HG2	2.17	0.45
1:A:520:MET:SD	1:A:608:VAL:HG12	2.57	0.44
1:A:355:GLU:O	1:A:611:ARG:NH2	2.49	0.44
1:B:444:ALA:HA	1:B:450:HIS:HD2	1.82	0.44
1:A:213:PHE:CE1	1:A:474:MET:HB2	2.52	0.44
1:B:153:ILE:HD11	1:B:250:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:HA	1:A:703:ARG:HE	1.81	0.44
1:A:98:LEU:HG	1:A:164:TRP:HB2	1.99	0.44
1:A:629:ILE:HG13	1:A:717:VAL:HG22	2.00	0.44
1:A:591:ALA:O	1:A:595:MET:HG2	2.17	0.44
1:A:642:VAL:HG21	1:A:700:SER:HB3	1.99	0.44
1:B:213:PHE:CZ	1:B:474:MET:HB3	2.53	0.44
1:B:568:PHE:CE2	1:B:604:LEU:HG	2.52	0.44
1:A:350:MET:HB3	1:A:350:MET:HE2	1.57	0.44
1:B:213:PHE:CE1	1:B:222:THR:HG22	2.51	0.44
1:B:706:ILE:CG2	3:B:6430:HOH:O	2.66	0.44
1:A:91:PRO:HB3	1:A:139:ASP:O	2.18	0.44
1:B:557:ILE:CD1	1:B:568:PHE:HB3	2.48	0.43
1:B:363:LYS:O	1:B:366:LYS:HD3	2.18	0.43
1:B:377:GLU:HB3	1:B:392:TRP:CE3	2.53	0.43
1:A:162:ALA:HB1	1:A:169:VAL:CG1	2.48	0.43
1:A:123:SER:O	1:A:133:LYS:HG3	2.18	0.43
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.50	0.43
1:B:90:ARG:NH1	1:B:97:ASP:OD2	2.52	0.43
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.53	0.43
1:B:104:VAL:HG12	1:B:116:TYR:HD1	1.84	0.43
1:A:549:ILE:CG2	1:A:550:THR:N	2.78	0.43
1:B:516:SER:N	1:B:617:ASP:OD2	2.52	0.43
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.73	0.43
1:B:557:ILE:HD12	1:B:568:PHE:HD2	1.83	0.43
1:A:697:PRO:HG3	1:A:725:ILE:HD12	2.00	0.43
1:B:44:PHE:O	1:B:45:LEU:CB	2.54	0.42
1:A:681:ARG:HH11	1:A:681:ARG:HG3	1.84	0.42
1:B:518:VAL:HB	1:B:612:ILE:HD11	2.01	0.42
1:A:51:HIS:HB3	3:A:6432:HOH:O	2.18	0.42
1:B:197:ASN:H	1:B:197:ASN:ND2	2.17	0.42
1:B:519:ASP:HB3	1:B:540:ARG:HD2	2.01	0.42
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.49	0.42
1:B:700:SER:HA	1:B:725:ILE:HG22	2.00	0.42
1:A:490:GLU:HG2	1:A:490:GLU:O	2.19	0.42
1:A:204:TYR:O	1:A:326:ARG:HG2	2.18	0.42
1:A:95:ARG:CG	1:A:96:ARG:HH11	2.32	0.42
1:B:650:VAL:HG11	1:B:667:LEU:HD13	2.01	0.42
1:B:557:ILE:HD12	1:B:568:PHE:CD2	2.54	0.42
1:A:636:VAL:HG12	1:A:648:VAL:HG22	2.01	0.42
1:B:353:PHE:CD2	1:B:364:LEU:HB3	2.54	0.42
1:A:639:THR:O	1:A:646:MET:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ILE:N	1:A:589:ILE:HD13	2.35	0.42
1:B:642:VAL:HG11	1:B:727:ARG:HH22	1.85	0.42
1:A:555:ALA:HA	1:A:605:HIS:O	2.20	0.42
1:B:641:VAL:HG22	1:B:726:GLN:HB2	2.01	0.42
1:A:662:ASN:HB2	1:A:712:ASP:OD1	2.20	0.42
1:B:565:LYS:HE2	1:B:565:LYS:HB3	1.71	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.81	0.42
1:B:237:THR:HG21	1:B:299:LEU:HB3	2.01	0.42
1:B:549:ILE:CG2	1:B:550:THR:N	2.82	0.42
1:A:187:TRP:NE1	1:A:201:ARG:HD2	2.34	0.42
1:B:440:ILE:HD12	1:B:440:ILE:HG23	1.71	0.42
1:A:310:ARG:HA	1:A:311:TYR:HA	1.91	0.42
1:B:472:ASP:OD2	1:B:704:LYS:NZ	2.53	0.41
1:A:678:LYS:HD2	1:A:691:TRP:NE1	2.35	0.41
1:B:642:VAL:HG11	1:B:727:ARG:NH2	2.35	0.41
1:B:187:TRP:CE2	1:B:201:ARG:HD3	2.55	0.41
1:B:556:ASN:HD22	1:B:567:GLU:HA	1.85	0.41
1:A:235:LEU:HA	1:A:327:CYS:SG	2.60	0.41
1:A:45:LEU:HD22	1:A:97:ASP:CG	2.40	0.41
1:A:193:VAL:HG13	1:A:331:PRO:HD3	2.01	0.41
1:A:303:ARG:HG2	3:A:6281:HOH:O	2.21	0.41
1:B:393:GLN:HB3	1:B:411:PRO:HB2	2.01	0.41
1:A:548:THR:HG22	1:A:576:THR:HG23	2.03	0.41
1:A:559:PHE:HB2	1:B:8:PHE:CE2	2.54	0.41
1:A:12:ARG:HH22	1:B:406:MET:HE1	1.86	0.41
1:A:77:ARG:HB3	1:A:185:ASN:HB2	2.02	0.41
1:A:194:TYR:HB3	3:A:6320:HOH:O	2.20	0.41
1:A:269:LYS:O	1:A:270:ASP:HB2	2.21	0.41
1:B:45:LEU:HG	1:B:88:PHE:CD1	2.56	0.41
1:A:313:GLN:OE1	1:A:315:TRP:HH2	2.04	0.40
1:B:611:ARG:HB3	1:B:611:ARG:HE	1.46	0.40
1:A:185:ASN:HD22	1:A:188:CYS:HB2	1.82	0.40
1:A:636:VAL:HG11	1:A:646:MET:CE	2.52	0.40
1:A:600:GLU:O	1:A:601:GLN:HB2	2.22	0.40
1:B:293:THR:HA	3:B:6430:HOH:O	2.20	0.40
1:B:197:ASN:H	1:B:197:ASN:HD22	1.68	0.40
1:B:341:ALA:HB2	1:B:460:ILE:HD13	2.03	0.40
1:B:137:ARG:CG	1:B:137:ARG:NH1	2.82	0.40
1:B:30:GLU:O	1:B:168:GLY:HA3	2.22	0.40
1:A:353:PHE:HA	1:A:442:ILE:O	2.22	0.40
1:A:186:PRO:HG2	1:A:205:VAL:HG21	2.03	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	695/731 (95%)	644 (93%)	44 (6%)	7 (1%)	19	13
1	B	701/731 (96%)	662 (94%)	34 (5%)	5 (1%)	26	21
All	All	1396/1462 (96%)	1306 (94%)	78 (6%)	12 (1%)	21	15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	B	45	LEU
1	A	281	ASN
1	A	270	ASP
1	A	196	ASP
1	A	681	ARG
1	A	711	SER
1	A	612	ILE
1	B	34	VAL
1	B	686	ASN
1	B	470	GLY
1	B	94	PRO

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	618/644 (96%)	570 (92%)	48 (8%)	16 11
1	B	621/644 (96%)	558 (90%)	63 (10%)	9 5
All	All	1239/1288 (96%)	1128 (91%)	111 (9%)	12 8

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	46	ASN
1	A	47	VAL
1	A	58	ASP
1	A	104	VAL
1	A	112	ASN
1	A	124	GLU
1	A	135	VAL
1	A	195	LEU
1	A	206	LEU
1	A	223	ARG
1	A	271	ASP
1	A	281	ASN
1	A	289	PRO
1	A	301	GLU
1	A	347	ASN
1	A	350	MET
1	A	354	LEU
1	A	364	LEU
1	A	368	SER
1	A	386	PRO
1	A	408	ARG
1	A	415	GLN
1	A	460	ILE
1	A	463	LEU
1	A	465	VAL
1	A	468	GLN
1	A	482	LYS
1	A	488	GLU
1	A	491	ARG
1	A	498	LEU
1	A	516	SER
1	A	523	GLU
1	A	525	GLU
1	A	534	LYS

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Mol	Chain	Res	Type
1	A	553	LEU
1	A	570	LYS
1	A	572	THR
1	A	587	VAL
1	A	597	GLN
1	A	604	LEU
1	A	616	ARG
1	A	625	THR
1	A	629	ILE
1	A	637	ARG
1	A	661	ARG
1	A	681	ARG
1	A	721	LEU
1	B	12	ARG
1	B	14	VAL
1	B	18	ASN
1	B	20	ASN
1	B	42	GLN
1	B	46	ASN
1	B	72	ASN
1	B	76	VAL
1	B	98	LEU
1	B	112	ASN
1	B	137	ARG
1	B	138	GLU
1	B	140	ARG
1	B	147	GLN
1	B	164	TRP
1	B	167	TYR
1	B	169	VAL
1	B	172	THR
1	B	174	ARG
1	B	195	LEU
1	B	206	LEU
1	B	223	ARG
1	B	235	LEU
1	B	239	LEU
1	B	304	SER
1	B	340	SER
1	B	359	ASN
1	B	408	ARG
1	B	451	VAL

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Mol	Chain	Res	Type
1	B	455	VAL
1	B	463	LEU
1	B	465	VAL
1	B	468	GLN
1	B	482	LYS
1	B	484	GLN
1	B	488	GLU
1	B	489	GLU
1	B	494	LEU
1	B	498	LEU
1	B	507	ASN
1	B	519	ASP
1	B	520	MET
1	B	531	LYS
1	B	538	THR
1	B	540	ARG
1	B	546	ARG
1	B	557	ILE
1	B	559	PHE
1	B	571	GLU
1	B	574	ASP
1	B	578	GLU
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	611	ARG
1	B	625	THR
1	B	626	VAL
1	B	637	ARG
1	B	639	THR
1	B	656	LEU
1	B	704	LYS
1	B	721	LEU
1	B	727	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	112	ASN
1	A	267	ASN
1	A	281	ASN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	526	ASN
1	A	597	GLN
1	A	605	HIS
1	A	622	GLN
1	B	18	ASN
1	B	72	ASN
1	B	112	ASN
1	B	359	ASN
1	B	450	HIS
1	B	468	GLN
1	B	484	GLN
1	B	545	ASN
1	B	556	ASN
1	B	613	ASN
1	B	662	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.