Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:32 PM GMT

PDB ID	:	1U3Q
Title	:	Crystal Structure of Estrogen Receptor beta complexed with CL-272
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Deposited on	:	2004-07-22
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

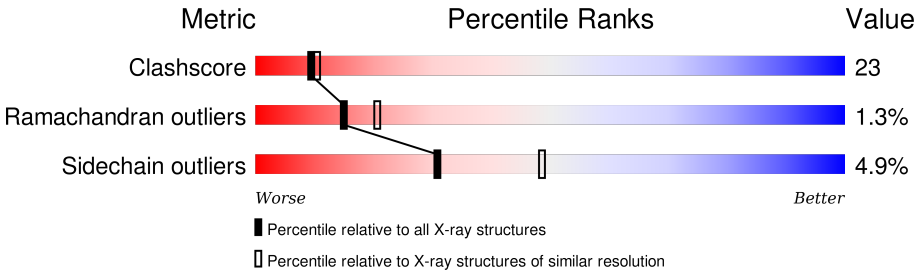
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 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	240	57% 33% 5% 6%
1	B	240	53% 38% • • 5%
1	C	240	57% 33% • 6%
1	D	240	64% 26% • 6%

2 Entry composition

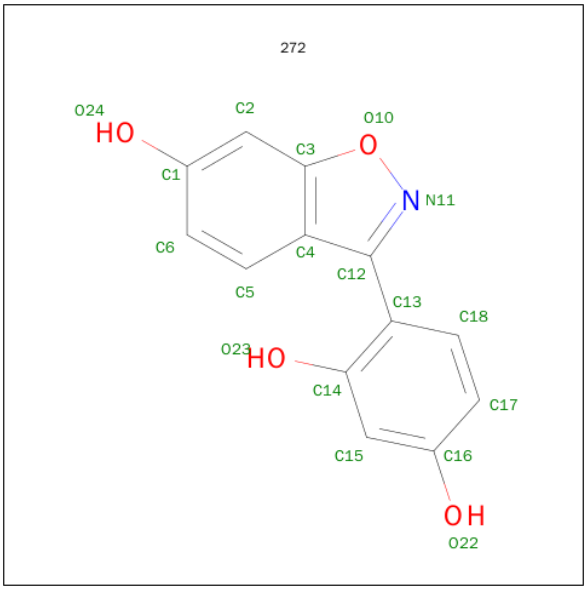
There are 3 unique types of molecules in this entry. The entry contains 7453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Estrogen receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1788	1150	300	318	20			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1148	301	320	20			
1	C	226	Total	C	N	O	S	0	0	0
			1788	1150	300	318	20			
1	D	226	Total	C	N	O	S	0	0	0
			1788	1150	300	318	20			

- Molecule 2 is 4-(6-HYDROXY-BENZO[D]ISOXAZOL-3-YL)BENZENE-1,3-DIOL (three-letter code: 272) (formula: $C_{13}H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	1	4		
2	B	1	Total	C	N	O	0	0
			18	13	1	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 18 13 1 4	0	0
2	D	1	Total C N O 18 13 1 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	65	Total O 65 65	0	0
3	C	38	Total O 38 38	0	0
3	D	62	Total O 62 62	0	0

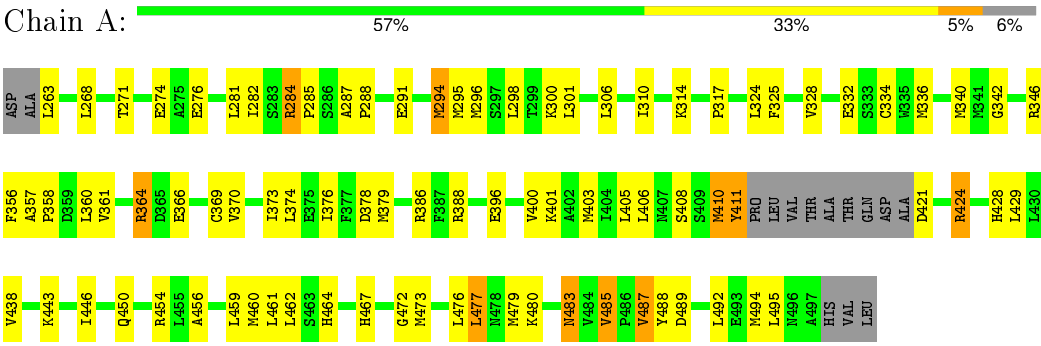
3 Residue-property plots (i)

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.

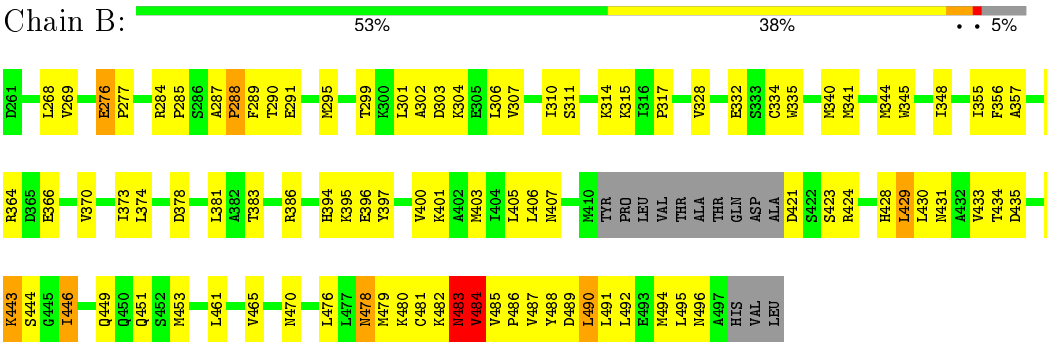
- Molecule 1: Estrogen receptor beta

Chain A:



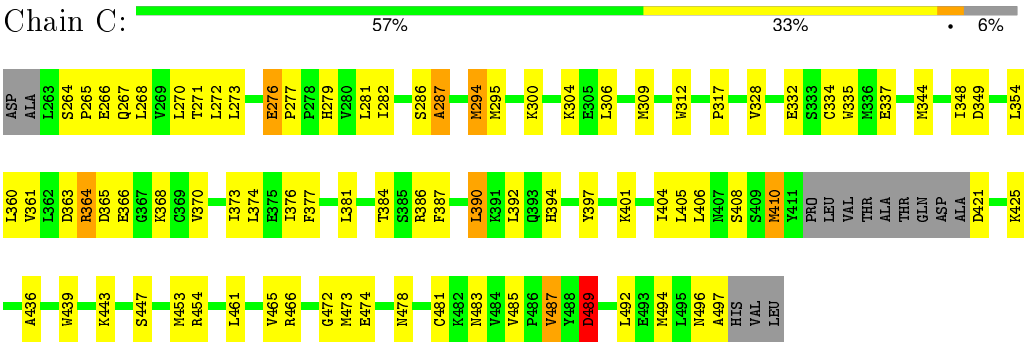
- Molecule 1: Estrogen receptor beta

Chain B:



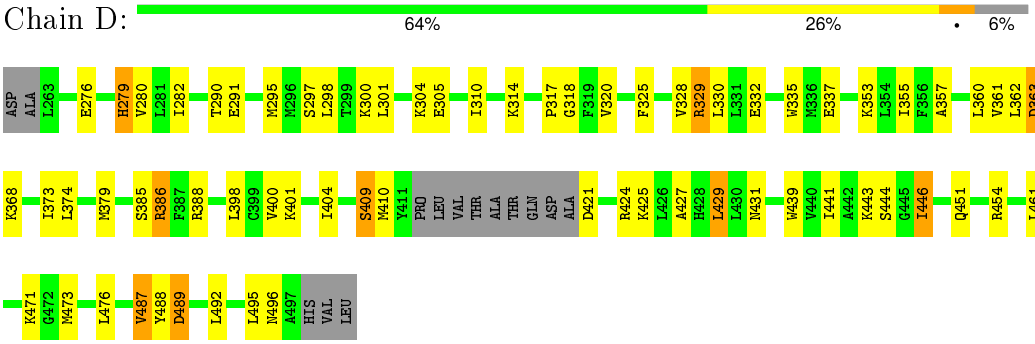
- Molecule 1: Estrogen receptor beta

Chain C:



• Molecule 1: Estrogen receptor beta

Chain D:



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	77.17Å 76.65Å 82.80Å 90.00° 111.83° 90.00°	Depositor
Resolution (Å)	14.95 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (14.95-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7453	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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: 272

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	0.36	0/1820	0.58	0/2456
1	B	0.35	0/1820	0.58	0/2456
1	C	0.40	1/1820 (0.1%)	0.57	0/2456
1	D	0.39	0/1820	0.60	0/2456
All	All	0.38	1/7280 (0.0%)	0.58	0/9824

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	478	ASN	C-N	6.99	1.50	1.34

There are no bond angle outliers.

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	1788	0	1864	94	0
1	B	1789	0	1864	102	0
1	C	1788	0	1864	82	0
1	D	1788	0	1864	74	0
2	A	18	0	6	0	0
2	B	18	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	18	0	6	0	0
2	D	18	0	6	1	0
3	A	63	0	0	3	0
3	B	65	0	0	4	0
3	C	38	0	0	3	0
3	D	62	0	0	4	0
All	All	7453	0	7480	332	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 23.

All (332) 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:B:478:ASN:ND2	1:B:482:LYS:HE3	1.47	1.27
1:B:478:ASN:HD21	1:B:482:LYS:CE	1.63	1.09
1:B:481:CYS:HB3	1:C:368:LYS:HE2	1.41	1.01
1:C:295:MET:HB3	1:C:485:VAL:HG21	1.51	0.92
1:A:477:LEU:HD13	1:A:495:LEU:HD22	1.53	0.89
1:B:478:ASN:C	1:B:478:ASN:HD22	1.75	0.89
1:A:376:ILE:HA	1:A:379:MET:HE2	1.56	0.88
1:B:434:THR:O	1:B:438:VAL:HG23	1.80	0.82
1:D:363:ASP:H	1:D:366:GLU:HG3	1.46	0.81
1:B:476:LEU:HG	1:B:495:LEU:HD11	1.64	0.80
1:A:476:LEU:HD23	1:A:495:LEU:HD21	1.63	0.80
1:B:478:ASN:HD21	1:B:482:LYS:HE3	0.70	0.78
1:C:487:VAL:HG11	1:C:492:LEU:HD13	1.63	0.77
1:A:467:HIS:HB2	1:C:466:ARG:HH11	1.48	0.77
1:C:267:GLN:HA	1:C:270:LEU:HD12	1.67	0.76
1:D:310:ILE:O	1:D:314:LYS:HG3	1.85	0.76
1:D:295:MET:HE3	1:D:373:ILE:HD12	1.68	0.75
1:D:353:LYS:HG2	1:D:363:ASP:OD1	1.87	0.73
1:B:306:LEU:HB2	1:B:490:LEU:HD12	1.67	0.73
1:B:383:THR:HA	1:D:410:MET:CE	2.18	0.73
1:B:303:ASP:OD1	1:B:490:LEU:HG	1.89	0.73
1:C:266:GLU:O	1:C:270:LEU:HG	1.88	0.73
1:D:363:ASP:H	1:D:366:GLU:CG	2.02	0.73
1:B:364:ARG:HG2	1:B:381:LEU:CD1	2.19	0.72
1:B:306:LEU:HD13	1:B:494:MET:HG3	1.72	0.71
1:A:406:LEU:CD1	1:A:429:LEU:HD22	2.20	0.71
1:B:364:ARG:HG2	1:B:381:LEU:HD13	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:HE2	1:B:362:LEU:HD21	1.56	0.71
1:A:479:MET:HB3	1:A:485:VAL:HG13	1.72	0.71
1:A:287:ALA:HB1	1:A:288:PRO:HD2	1.72	0.70
1:B:386:ARG:NH1	1:D:410:MET:HA	2.06	0.70
1:A:334:CYS:HB3	1:A:408:SER:CB	2.22	0.70
1:A:364:ARG:HD3	1:A:378:ASP:OD1	1.92	0.70
1:D:317:PRO:O	1:D:429:LEU:HD21	1.92	0.69
1:B:341:MET:HA	1:B:344:MET:HE2	1.73	0.69
1:B:340:MET:O	1:B:344:MET:HG3	1.93	0.69
1:C:286:SER:HA	3:C:172:HOH:O	1.93	0.69
1:A:473:MET:HE3	1:A:495:LEU:HD23	1.75	0.69
1:D:282:ILE:HD13	1:D:360:LEU:HD22	1.74	0.68
1:B:442:ALA:HA	1:B:451:GLN:OE1	1.93	0.68
1:B:328:VAL:O	1:B:332:GLU:HG3	1.94	0.68
1:A:295:MET:HE2	1:A:370:VAL:HG21	1.75	0.67
1:A:334:CYS:HB3	1:A:408:SER:HB3	1.76	0.67
1:A:328:VAL:O	1:A:332:GLU:HG3	1.95	0.67
1:C:300:LYS:O	1:C:304:LYS:HG3	1.96	0.66
1:A:376:ILE:HD13	1:A:472:GLY:HA2	1.78	0.66
1:B:478:ASN:C	1:B:478:ASN:ND2	2.49	0.65
1:B:289:PHE:CE2	1:B:362:LEU:HD21	2.30	0.65
1:A:306:LEU:HD13	1:A:494:MET:HG3	1.78	0.65
1:B:364:ARG:HD3	1:B:378:ASP:OD1	1.96	0.65
1:D:425:LYS:O	1:D:429:LEU:HB2	1.95	0.65
1:D:487:VAL:HG23	1:D:492:LEU:HB2	1.79	0.65
1:B:295:MET:HE3	1:B:370:VAL:HG11	1.80	0.64
1:D:364:ARG:HH21	1:D:374:LEU:HD11	1.62	0.64
1:B:480:LYS:HB2	1:B:487:VAL:HG23	1.79	0.64
1:B:364:ARG:CZ	1:B:374:LEU:HD11	2.28	0.64
1:C:376:ILE:HD13	1:C:472:GLY:HA2	1.78	0.64
1:A:421:ASP:HA	1:A:424:ARG:NH1	2.13	0.64
1:A:294:MET:HE2	1:A:369:CYS:HB2	1.80	0.63
1:B:428:HIS:HB2	3:B:37:HOH:O	1.98	0.63
1:D:488:TYR:O	1:D:492:LEU:HB3	1.99	0.63
1:B:386:ARG:HH12	1:D:410:MET:HA	1.62	0.62
1:A:428:HIS:HB2	3:A:92:HOH:O	1.99	0.62
1:B:490:LEU:HD23	1:B:490:LEU:H	1.63	0.62
1:C:295:MET:HB3	1:C:485:VAL:CG2	2.24	0.62
1:C:276:GLU:OE1	1:C:276:GLU:HA	1.99	0.62
1:A:271:THR:HG21	1:A:317:PRO:HG3	1.82	0.62
1:C:273:LEU:HD13	1:C:394:HIS:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:NZ	1:C:368:LYS:HB2	2.15	0.62
1:B:444:SER:OG	1:B:446:ILE:HG12	2.00	0.62
1:A:406:LEU:HD13	1:A:429:LEU:HD22	1.81	0.61
1:C:364:ARG:C	1:C:364:ARG:HD2	2.20	0.61
1:A:295:MET:HB3	1:A:485:VAL:HG12	1.81	0.61
1:C:334:CYS:HB3	1:C:408:SER:CB	2.31	0.61
1:C:406:LEU:HB2	1:C:430:LEU:HD13	1.82	0.61
1:C:368:LYS:HG2	1:C:374:LEU:HD22	1.82	0.61
1:A:295:MET:HE3	1:A:370:VAL:HG11	1.81	0.61
1:D:337:GLU:OE2	1:D:466:ARG:NE	2.34	0.60
1:C:481:CYS:C	1:C:483:ASN:H	2.02	0.60
1:D:300:LYS:O	1:D:304:LYS:HG3	2.01	0.60
1:A:370:VAL:HB	1:A:373:ILE:CG2	2.32	0.60
1:A:336:MET:O	1:A:340:MET:HG3	2.00	0.60
1:B:476:LEU:HD23	1:B:495:LEU:HD21	1.83	0.59
1:A:406:LEU:HD11	1:A:429:LEU:HD22	1.83	0.59
1:B:383:THR:HA	1:D:410:MET:HE3	1.84	0.59
1:A:473:MET:CE	1:A:495:LEU:HD23	2.33	0.59
1:C:355:ILE:HD13	1:C:361:VAL:HG13	1.84	0.59
1:A:295:MET:CB	1:A:485:VAL:HG12	2.33	0.59
1:A:295:MET:CG	1:A:485:VAL:HG12	2.32	0.59
1:A:334:CYS:SG	1:A:405:LEU:HD12	2.42	0.59
1:C:286:SER:O	1:C:287:ALA:HB2	2.02	0.59
1:D:386:ARG:NE	3:D:80:HOH:O	2.36	0.58
1:A:434:THR:O	1:A:438:VAL:HG23	2.04	0.58
1:B:421:ASP:HA	1:B:424:ARG:NH1	2.19	0.58
1:B:481:CYS:HB3	1:C:368:LYS:CE	2.27	0.58
1:D:476:LEU:HD23	1:D:495:LEU:HD21	1.84	0.58
1:C:267:GLN:O	1:C:271:THR:HG23	2.03	0.57
1:B:310:ILE:O	1:B:314:LYS:HG3	2.04	0.57
1:B:284:ARG:HG2	1:B:285:PRO:HD2	1.87	0.57
1:A:274:GLU:HG3	3:A:219:HOH:O	2.04	0.57
1:D:421:ASP:HA	1:D:424:ARG:NH1	2.20	0.56
1:A:296:MET:O	1:A:300:LYS:HB2	2.04	0.56
1:B:334:CYS:SG	1:B:405:LEU:HD12	2.44	0.56
1:D:386:ARG:HG2	1:D:461:LEU:HD21	1.86	0.56
1:A:295:MET:HG3	1:A:485:VAL:HG12	1.86	0.56
1:B:480:LYS:NZ	1:C:364:ARG:HH22	2.04	0.56
1:B:489:ASP:OD2	1:B:490:LEU:HD23	2.05	0.56
1:C:281:LEU:HD22	1:C:281:LEU:N	2.20	0.56
1:A:268:LEU:CD1	1:A:317:PRO:HG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:MET:CE	1:B:373:ILE:HD12	2.36	0.55
1:A:483:ASN:HB3	1:D:365:ASP:OD1	2.06	0.55
1:A:467:HIS:HB2	1:C:466:ARG:NH1	2.19	0.55
1:B:488:TYR:O	1:B:492:LEU:HB2	2.06	0.55
1:B:295:MET:HE3	1:B:373:ILE:HD12	1.89	0.55
1:D:427:ALA:O	1:D:431:ASN:HB2	2.06	0.55
1:B:287:ALA:HB1	1:B:288:PRO:CD	2.37	0.55
1:A:295:MET:CE	1:A:370:VAL:HG11	2.37	0.55
1:A:294:MET:HE1	1:A:366:GLU:O	2.07	0.55
1:C:295:MET:CB	1:C:485:VAL:HG21	2.33	0.55
1:D:295:MET:HE1	1:D:298:LEU:HD12	1.90	0.54
1:B:355:ILE:HD13	1:B:361:VAL:HG13	1.89	0.54
1:D:301:LEU:O	1:D:305:GLU:HG3	2.07	0.54
1:C:443:LYS:HB3	1:C:443:LYS:NZ	2.22	0.54
1:A:310:ILE:O	1:A:314:LYS:HG3	2.08	0.54
1:C:487:VAL:HB	1:C:492:LEU:HB2	1.90	0.54
1:C:496:ASN:O	1:C:497:ALA:C	2.45	0.53
1:B:307:VAL:HG23	1:B:490:LEU:HD11	1.89	0.53
1:B:439:TRP:CE2	1:B:443:LYS:HD3	2.43	0.53
1:A:485:VAL:HG23	1:A:487:VAL:HG13	1.89	0.53
1:A:396:GLU:CD	1:A:454:ARG:HH21	2.11	0.53
1:B:481:CYS:SG	1:C:368:LYS:HD3	2.49	0.53
1:C:295:MET:HE3	1:C:370:VAL:HG11	1.90	0.53
1:D:487:VAL:HG22	1:D:492:LEU:HD13	1.89	0.53
1:B:443:LYS:NZ	1:B:443:LYS:HA	2.23	0.53
1:B:406:LEU:CD2	1:B:429:LEU:HD22	2.38	0.53
1:D:487:VAL:CG2	1:D:492:LEU:HD13	2.38	0.53
1:C:387:PHE:CD1	1:C:392:LEU:HD22	2.44	0.53
1:A:400:VAL:HG13	1:A:462:LEU:HD21	1.91	0.53
1:C:489:ASP:OD2	1:C:489:ASP:N	2.42	0.52
1:B:383:THR:HA	1:D:410:MET:HE1	1.90	0.52
1:C:363:ASP:O	1:C:366:GLU:HB2	2.09	0.52
1:B:276:GLU:HA	1:B:276:GLU:OE1	2.09	0.52
1:C:306:LEU:HD13	1:C:494:MET:HG3	1.92	0.52
1:A:479:MET:HB3	1:A:485:VAL:CG1	2.38	0.52
1:A:456:ALA:O	1:A:460:MET:HG3	2.08	0.52
1:A:296:MET:SD	1:A:300:LYS:HD2	2.50	0.52
1:D:276:GLU:HG2	1:D:398:LEU:HD21	1.90	0.52
1:D:362:LEU:HA	1:D:366:GLU:HG3	1.92	0.52
1:D:328:VAL:O	1:D:332:GLU:HG3	2.09	0.52
1:A:306:LEU:O	1:A:310:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HG3	1:A:461:LEU:HD11	1.91	0.52
1:A:364:ARG:NH1	1:A:374:LEU:HD11	2.25	0.52
1:A:386:ARG:HG2	1:A:461:LEU:HD21	1.91	0.52
1:D:488:TYR:O	1:D:492:LEU:CB	2.58	0.51
1:B:269:VAL:HG11	1:B:395:LYS:HD3	1.91	0.51
1:A:370:VAL:HB	1:A:373:ILE:HG22	1.92	0.51
1:B:487:VAL:HG13	1:B:491:LEU:HD23	1.92	0.51
1:B:423:SER:HB2	3:B:15:HOH:O	2.10	0.51
1:B:449:GLN:NE2	1:B:453:MET:CE	2.73	0.51
1:C:370:VAL:HB	1:C:373:ILE:CG2	2.41	0.51
1:C:364:ARG:HG2	1:C:381:LEU:CD1	2.41	0.51
1:B:476:LEU:CG	1:B:495:LEU:HD11	2.39	0.50
1:B:306:LEU:CB	1:B:490:LEU:HD12	2.41	0.50
1:A:480:LYS:HG3	3:D:17:HOH:O	2.11	0.50
1:C:306:LEU:HD21	1:C:335:TRP:HB2	1.93	0.50
1:B:304:LYS:HE3	3:B:175:HOH:O	2.11	0.50
1:A:410:MET:O	1:A:411:TYR:C	2.49	0.50
1:A:431:ASN:OD1	1:C:453:MET:SD	2.69	0.50
1:D:280:VAL:HG21	1:D:305:GLU:HG2	1.93	0.50
1:B:364:ARG:NH1	1:B:374:LEU:HD11	2.26	0.50
1:C:370:VAL:HB	1:C:373:ILE:HG21	1.92	0.50
1:A:294:MET:CE	1:A:370:VAL:HG23	2.41	0.50
1:C:481:CYS:C	1:C:483:ASN:N	2.65	0.50
1:C:268:LEU:O	1:C:272:LEU:HG	2.11	0.50
1:B:276:GLU:OE1	1:B:277:PRO:HD2	2.12	0.49
1:A:488:TYR:O	1:A:492:LEU:HB2	2.11	0.49
1:B:295:MET:O	1:B:299:THR:HG23	2.12	0.49
1:C:454:ARG:HG3	1:C:454:ARG:HH11	1.78	0.49
1:D:363:ASP:N	1:D:366:GLU:HG3	2.22	0.49
1:B:355:ILE:HD12	1:B:361:VAL:HG22	1.94	0.49
1:C:443:LYS:HE3	3:C:69:HOH:O	2.11	0.49
1:D:276:GLU:CG	1:D:398:LEU:HD21	2.43	0.49
1:A:263:LEU:N	3:A:75:HOH:O	2.45	0.49
1:C:294:MET:HE2	1:C:370:VAL:HG23	1.94	0.49
1:B:480:LYS:HZ1	1:C:364:ARG:HH22	1.60	0.49
1:B:284:ARG:HG2	1:B:285:PRO:CD	2.42	0.49
1:D:364:ARG:HH21	1:D:374:LEU:CD1	2.26	0.49
1:A:324:LEU:HG	1:B:328:VAL:CG2	2.43	0.48
1:B:287:ALA:HB1	1:B:288:PRO:HD2	1.95	0.48
1:D:282:ILE:HD13	1:D:360:LEU:CD2	2.41	0.48
1:C:397:TYR:CZ	1:C:401:LYS:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LEU:HD12	1:C:268:LEU:O	2.14	0.48
1:C:334:CYS:HB3	1:C:408:SER:HB3	1.94	0.48
1:B:443:LYS:HA	1:B:443:LYS:HZ3	1.78	0.48
1:B:268:LEU:CD1	1:B:317:PRO:HG2	2.43	0.48
1:D:357:ALA:HB3	1:D:360:LEU:HB3	1.95	0.48
1:B:304:LYS:HG2	3:B:175:HOH:O	2.13	0.48
1:B:290:THR:O	1:B:291:GLU:C	2.51	0.48
1:C:273:LEU:O	1:C:276:GLU:HB2	2.14	0.47
1:C:429:LEU:O	1:C:433:VAL:HG23	2.14	0.47
1:C:337:GLU:HB3	1:C:404:ILE:HG21	1.95	0.47
1:B:301:LEU:CD2	1:B:356:PHE:HB3	2.45	0.47
1:D:325:PHE:O	1:D:329:ARG:HB2	2.13	0.47
1:A:488:TYR:O	1:A:492:LEU:CB	2.63	0.47
1:B:345:TRP:O	1:B:348:ILE:HG22	2.15	0.47
1:C:410:MET:HG2	1:C:410:MET:H	1.54	0.47
1:C:276:GLU:CD	1:C:277:PRO:HD2	2.35	0.47
1:D:439:TRP:O	1:D:443:LYS:HG2	2.14	0.47
1:D:318:GLY:C	1:D:429:LEU:HD11	2.35	0.46
1:D:386:ARG:CG	1:D:461:LEU:HD21	2.45	0.46
1:B:397:TYR:CZ	1:B:401:LYS:HE2	2.48	0.46
1:A:306:LEU:CD1	1:A:494:MET:HG3	2.45	0.46
1:C:282:ILE:HG22	1:C:357:ALA:CB	2.45	0.46
1:A:325:PHE:CD2	1:B:328:VAL:HG13	2.51	0.46
1:C:461:LEU:O	1:C:465:VAL:HG23	2.16	0.46
1:A:446:ILE:HD12	1:A:450:GLN:HB3	1.95	0.46
1:A:485:VAL:CG2	1:A:487:VAL:HG13	2.46	0.46
1:B:302:ALA:O	1:B:306:LEU:HG	2.15	0.46
1:A:295:MET:HE1	1:A:298:LEU:HD12	1.98	0.46
1:C:377:PHE:O	1:C:381:LEU:HG	2.15	0.46
1:C:273:LEU:CD1	1:C:394:HIS:HE1	2.29	0.46
1:D:279:HIS:ND1	1:D:279:HIS:N	2.64	0.46
1:B:396:GLU:O	1:B:400:VAL:HG23	2.16	0.46
1:C:404:ILE:O	1:C:408:SER:HB3	2.15	0.46
1:B:268:LEU:HD13	1:B:317:PRO:HG2	1.98	0.46
1:A:443:LYS:HB3	1:A:443:LYS:NZ	2.31	0.46
1:A:282:ILE:HG22	1:A:357:ALA:CB	2.46	0.46
1:A:410:MET:HB3	3:C:227:HOH:O	2.15	0.45
1:D:305:GLU:OE2	2:D:501:272:O24	2.35	0.45
1:A:386:ARG:HD2	1:A:386:ARG:HA	1.56	0.45
1:B:344:MET:HE1	1:B:465:VAL:HG22	1.98	0.45
1:A:342:GLY:O	1:A:346:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ASP:H	1:B:366:GLU:HG3	1.80	0.45
1:D:385:SER:HA	1:D:388:ARG:NH1	2.32	0.45
1:B:276:GLU:CD	1:B:277:PRO:HD2	2.36	0.45
1:D:401:LYS:HD3	3:D:23:HOH:O	2.15	0.45
1:A:355:ILE:HD13	1:A:361:VAL:HG13	1.98	0.45
1:A:276:GLU:OE1	1:A:401:LYS:NZ	2.42	0.45
1:A:294:MET:HE2	1:A:370:VAL:HG23	1.99	0.45
1:B:439:TRP:O	1:B:443:LYS:HG2	2.17	0.45
1:B:403:MET:HG3	1:B:433:VAL:CG1	2.46	0.45
1:B:306:LEU:HD21	1:B:335:TRP:CE3	2.52	0.44
1:A:324:LEU:HG	1:B:328:VAL:HG22	1.98	0.44
1:A:268:LEU:HD12	1:A:317:PRO:HG2	1.99	0.44
1:C:357:ALA:HB3	1:C:360:LEU:HB3	1.98	0.44
1:C:421:ASP:O	1:C:425:LYS:HG2	2.16	0.44
1:C:390:LEU:HD22	1:C:454:ARG:NH1	2.33	0.44
1:B:295:MET:CE	1:B:370:VAL:HG21	2.48	0.44
1:C:276:GLU:OE1	1:C:277:PRO:HD2	2.18	0.44
1:D:304:LYS:HE2	1:D:304:LYS:HB3	1.83	0.44
1:D:295:MET:CE	1:D:373:ILE:HD12	2.42	0.44
1:C:286:SER:O	1:C:287:ALA:CB	2.66	0.43
1:D:282:ILE:HD12	1:D:297:SER:O	2.17	0.43
1:B:492:LEU:CD1	1:B:496:ASN:HD21	2.31	0.43
1:B:394:HIS:O	1:B:397:TYR:HB3	2.18	0.43
1:A:282:ILE:HG22	1:A:357:ALA:HB3	2.00	0.43
1:C:368:LYS:HZ2	1:C:368:LYS:HB2	1.83	0.43
1:B:483:ASN:ND2	1:C:365:ASP:OD2	2.51	0.43
1:A:476:LEU:HG	1:A:495:LEU:HD11	2.00	0.43
1:A:376:ILE:CD1	1:A:472:GLY:HA2	2.47	0.43
1:A:477:LEU:HD12	1:A:477:LEU:HA	1.90	0.43
1:D:363:ASP:O	1:D:365:ASP:N	2.52	0.43
1:C:386:ARG:HD2	1:C:386:ARG:HA	1.76	0.43
1:D:444:SER:OG	1:D:446:ILE:HG12	2.18	0.43
1:B:484:VAL:HG23	1:B:485:VAL:H	1.82	0.43
1:A:284:ARG:HG3	1:A:285:PRO:HD2	2.00	0.43
1:D:353:LYS:HD2	1:D:361:VAL:CG1	2.49	0.43
1:D:280:VAL:CG2	1:D:305:GLU:HG2	2.48	0.43
1:D:379:MET:CE	1:D:471:LYS:HG3	2.49	0.43
1:C:309:MET:O	1:C:312:TRP:HB3	2.18	0.43
1:D:355:ILE:O	1:D:355:ILE:HG22	2.19	0.43
1:C:344:MET:HG2	1:C:384:THR:OG1	2.18	0.43
1:A:351:PRO:HB3	1:A:388:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:TRP:HE1	1:D:473:MET:HE1	1.84	0.43
1:D:492:LEU:HD11	1:D:496:ASN:HD21	1.84	0.42
1:A:483:ASN:HD21	1:D:368:LYS:HB3	1.84	0.42
1:B:386:ARG:CD	1:B:461:LEU:HD21	2.49	0.42
2:B:501:272:H18	2:B:501:272:H5	2.01	0.42
1:B:311:SER:O	1:B:315:LYS:HG3	2.19	0.42
1:B:357:ALA:HB3	1:B:360:LEU:HB3	2.01	0.42
1:A:334:CYS:HB3	1:A:408:SER:HB2	2.00	0.42
1:C:454:ARG:HG3	1:C:454:ARG:NH1	2.34	0.42
1:B:403:MET:HG3	1:B:433:VAL:HG12	2.02	0.42
1:D:400:VAL:O	1:D:404:ILE:HG13	2.19	0.42
1:D:353:LYS:HD2	1:D:361:VAL:HG11	2.00	0.42
1:A:291:GLU:HG3	1:A:370:VAL:HA	2.02	0.42
1:D:421:ASP:HA	1:D:424:ARG:CZ	2.50	0.42
1:C:439:TRP:O	1:C:443:LYS:HG2	2.20	0.42
1:A:454:ARG:HH11	1:A:454:ARG:HG3	1.83	0.42
1:D:363:ASP:C	1:D:365:ASP:N	2.72	0.42
1:A:421:ASP:HA	1:A:424:ARG:HD3	2.00	0.42
1:C:264:SER:OG	1:C:267:GLN:HG2	2.19	0.42
1:A:294:MET:O	1:A:298:LEU:HG	2.20	0.42
1:B:344:MET:CE	1:B:465:VAL:HG22	2.50	0.42
1:D:454:ARG:HG3	1:D:454:ARG:HH11	1.84	0.42
1:C:354:LEU:HG	1:C:381:LEU:HD21	2.02	0.42
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.89	0.42
1:D:290:THR:O	1:D:291:GLU:C	2.58	0.42
1:B:355:ILE:HG23	1:B:361:VAL:HG22	2.02	0.41
1:C:282:ILE:HG22	1:C:357:ALA:HB2	2.02	0.41
1:B:470:ASN:HA	1:B:470:ASN:HD22	1.63	0.41
1:A:295:MET:HE3	1:A:373:ILE:HD12	2.01	0.41
1:B:406:LEU:HB2	1:B:430:LEU:HD13	2.02	0.41
1:D:320:VAL:HG22	3:D:77:HOH:O	2.19	0.41
1:A:485:VAL:O	1:A:485:VAL:CG2	2.68	0.41
1:B:407:ASN:O	1:D:464:HIS:CE1	2.74	0.41
1:D:276:GLU:OE1	1:D:401:LYS:NZ	2.44	0.41
1:C:317:PRO:O	1:C:429:LEU:HD21	2.21	0.41
1:A:356:PHE:HB2	1:A:360:LEU:HD23	2.01	0.41
1:D:363:ASP:C	1:D:365:ASP:H	2.24	0.41
1:C:334:CYS:SG	1:C:405:LEU:HD12	2.60	0.41
1:D:335:TRP:HZ2	1:D:473:MET:HE3	1.85	0.41
1:C:328:VAL:O	1:C:332:GLU:HG3	2.20	0.41
1:A:461:LEU:HA	1:A:464:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:CD2	1:A:356:PHE:HB3	2.49	0.41
1:D:330:LEU:CD2	1:D:409:SER:HB3	2.51	0.41
1:C:334:CYS:SG	1:C:405:LEU:CD1	3.08	0.41
1:A:282:ILE:HG21	1:A:360:LEU:HD22	2.02	0.41
1:B:386:ARG:HD3	1:B:461:LEU:HD21	2.02	0.41
1:A:403:MET:HE1	1:A:459:LEU:HD21	2.03	0.41
1:D:295:MET:CE	1:D:298:LEU:HD12	2.51	0.41
1:D:282:ILE:HD11	1:D:297:SER:HB3	2.03	0.41
1:D:476:LEU:HG	1:D:495:LEU:HD11	2.02	0.40
1:C:265:PRO:HB3	1:C:436:ALA:HA	2.03	0.40
1:A:281:LEU:HD23	1:A:358:PRO:HD2	2.03	0.40
1:B:406:LEU:CD1	1:B:429:LEU:HD22	2.52	0.40
1:D:441:ILE:HG22	1:D:451:GLN:HG2	2.03	0.40
1:B:461:LEU:HA	1:B:461:LEU:HD23	1.98	0.40
1:C:348:ILE:HG23	1:C:349:ASP:N	2.36	0.40
1:B:479:MET:HE2	1:B:482:LYS:NZ	2.36	0.40
1:A:467:HIS:CB	1:C:466:ARG:HH11	2.27	0.40
1:C:386:ARG:HG2	1:C:461:LEU:HD21	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	222/240 (92%)	205 (92%)	15 (7%)	2 (1%)	21	30
1	B	223/240 (93%)	206 (92%)	13 (6%)	4 (2%)	11	13
1	C	222/240 (92%)	209 (94%)	10 (4%)	3 (1%)	14	19
1	D	222/240 (92%)	215 (97%)	4 (2%)	3 (1%)	14	19
All	All	889/960 (93%)	835 (94%)	42 (5%)	12 (1%)	15	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP
1	B	446	ILE
1	B	484	VAL
1	D	446	ILE
1	B	483	ASN
1	C	489	ASP
1	D	364	ARG
1	D	489	ASP
1	C	447	SER
1	C	287	ALA
1	A	487	VAL
1	B	288	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	204/215 (95%)	194 (95%)	10 (5%)	31	48
1	B	204/215 (95%)	195 (96%)	9 (4%)	35	53
1	C	204/215 (95%)	192 (94%)	12 (6%)	24	38
1	D	204/215 (95%)	195 (96%)	9 (4%)	35	53
All	All	816/860 (95%)	776 (95%)	40 (5%)	31	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	ARG
1	A	294	MET
1	A	364	ARG
1	A	410	MET
1	A	411	TYR
1	A	424	ARG
1	A	431	ASN
1	A	477	LEU
1	A	483	ASN
1	A	485	VAL

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Mol	Chain	Res	Type
1	B	276	GLU
1	B	429	LEU
1	B	431	ASN
1	B	435	ASP
1	B	443	LYS
1	B	478	ASN
1	B	483	ASN
1	B	484	VAL
1	B	490	LEU
1	C	276	GLU
1	C	279	HIS
1	C	294	MET
1	C	359	ASP
1	C	364	ARG
1	C	390	LEU
1	C	410	MET
1	C	429	LEU
1	C	473	MET
1	C	474	GLU
1	C	487	VAL
1	C	489	ASP
1	D	279	HIS
1	D	329	ARG
1	D	363	ASP
1	D	364	ARG
1	D	386	ARG
1	D	409	SER
1	D	429	LEU
1	D	487	VAL
1	D	489	ASP

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

Mol	Chain	Res	Type
1	A	407	ASN
1	A	449	GLN
1	A	467	HIS
1	A	478	ASN
1	A	496	ASN
1	B	407	ASN
1	B	431	ASN
1	B	449	GLN

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Mol	Chain	Res	Type
1	B	470	ASN
1	B	478	ASN
1	B	483	ASN
1	B	496	ASN
1	C	267	GLN
1	C	394	HIS
1	C	449	GLN
1	C	467	HIS
1	C	470	ASN
1	C	478	ASN
1	D	267	GLN
1	D	449	GLN
1	D	464	HIS
1	D	470	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

4 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	272	A	501	-	16,20,20	3.68	14 (87%)	20,29,29	1.38	3 (15%)
2	272	B	501	-	16,20,20	3.47	13 (81%)	20,29,29	1.25	3 (15%)
2	272	C	501	-	16,20,20	3.55	11 (68%)	20,29,29	1.46	4 (20%)
2	272	D	501	-	16,20,20	3.52	10 (62%)	20,29,29	1.42	3 (15%)

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	272	A	501	-	-	0/2/4/4	0/2/3/3
2	272	B	501	-	-	0/2/4/4	0/2/3/3
2	272	C	501	-	-	0/2/4/4	0/2/3/3
2	272	D	501	-	-	0/2/4/4	0/2/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	272	O23-C14	-6.50	1.23	1.36
2	C	501	272	O23-C14	-6.49	1.23	1.36
2	D	501	272	O23-C14	-6.48	1.23	1.36
2	B	501	272	O23-C14	-6.40	1.23	1.36
2	C	501	272	O24-C1	-6.00	1.22	1.37
2	D	501	272	O24-C1	-5.99	1.22	1.37
2	B	501	272	O24-C1	-5.53	1.23	1.37
2	B	501	272	O22-C16	-5.53	1.23	1.37
2	A	501	272	O22-C16	-5.45	1.24	1.37
2	A	501	272	O24-C1	-5.41	1.24	1.37
2	C	501	272	O22-C16	-5.36	1.24	1.37
2	D	501	272	O22-C16	-4.92	1.25	1.37
2	B	501	272	C2-C3	2.01	1.41	1.37
2	A	501	272	C18-C13	2.07	1.43	1.39
2	A	501	272	C2-C3	2.21	1.42	1.37
2	B	501	272	C18-C13	2.22	1.43	1.39
2	C	501	272	C18-C13	2.35	1.43	1.39
2	D	501	272	C2-C1	2.35	1.41	1.37
2	D	501	272	C17-C16	2.44	1.43	1.38
2	A	501	272	C5-C4	2.46	1.47	1.42
2	B	501	272	C17-C16	2.58	1.44	1.38
2	B	501	272	C2-C1	2.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	272	C17-C16	2.75	1.44	1.38
2	B	501	272	C15-C14	2.84	1.42	1.38
2	A	501	272	C17-C16	2.89	1.44	1.38
2	A	501	272	C2-C1	2.90	1.42	1.37
2	A	501	272	C12-N11	2.95	1.38	1.33
2	C	501	272	C15-C14	2.96	1.43	1.38
2	B	501	272	C13-C12	2.98	1.52	1.49
2	C	501	272	C6-C1	3.09	1.45	1.38
2	B	501	272	C18-C17	3.11	1.44	1.38
2	B	501	272	C6-C1	3.14	1.45	1.38
2	B	501	272	C12-N11	3.15	1.39	1.33
2	C	501	272	C12-N11	3.19	1.39	1.33
2	A	501	272	C15-C14	3.21	1.43	1.38
2	C	501	272	C18-C17	3.38	1.44	1.38
2	A	501	272	C13-C12	3.47	1.53	1.49
2	D	501	272	C12-N11	3.53	1.39	1.33
2	C	501	272	C13-C12	3.62	1.53	1.49
2	D	501	272	C6-C1	3.63	1.46	1.38
2	D	501	272	C18-C17	3.66	1.45	1.38
2	A	501	272	C18-C17	3.68	1.45	1.38
2	D	501	272	C5-C6	3.80	1.44	1.36
2	B	501	272	C5-C6	3.80	1.44	1.36
2	A	501	272	C6-C1	3.80	1.46	1.38
2	D	501	272	C15-C14	3.82	1.44	1.38
2	C	501	272	C5-C6	4.07	1.45	1.36
2	A	501	272	C5-C6	4.25	1.45	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	272	C1-C2-C3	-3.31	117.37	120.42
2	C	501	272	C1-C2-C3	-3.18	117.49	120.42
2	B	501	272	C1-C2-C3	-3.15	117.52	120.42
2	C	501	272	C5-C4-C3	-3.03	118.62	120.33
2	A	501	272	C1-C2-C3	-2.93	117.72	120.42
2	A	501	272	C5-C4-C3	-2.89	118.70	120.33
2	B	501	272	C5-C4-C3	-2.45	118.95	120.33
2	D	501	272	C5-C4-C3	-2.34	119.01	120.33
2	C	501	272	C6-C5-C4	-2.28	118.14	121.13
2	D	501	272	C6-C5-C4	-2.24	118.19	121.13
2	A	501	272	C6-C5-C4	-2.09	118.39	121.13
2	B	501	272	C6-C5-C4	-2.08	118.40	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	272	C2-C3-C4	2.08	124.11	120.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	272	1	0
2	D	501	272	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 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.