



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 04:55 PM UTC

PDB ID : 1NBW / pdb_00001nbw
Title : Glycerol dehydratase reactivase
Authors : Liao, D.-I.; Reiss, L.; Turner Jr., I.; Dotson, G.
Deposited on : 2002-12-04
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
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

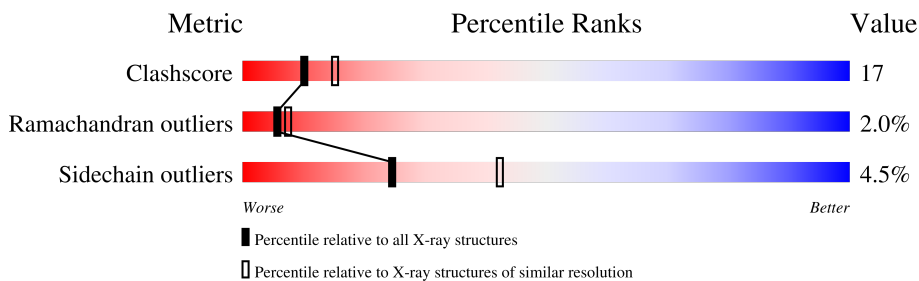
1 Overall quality at a glance

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	607	 75% 20% .
1	C	607	 66% 29% . .
2	B	117	 73% 21% . . .
2	D	117	 69% 25% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11079 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 GLYCEROL DEHYDRATASE REACTIVASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	0	0	0
			4452	2804	776	851	21			
1	C	604	Total	C	N	O	S	0	0	0
			4436	2795	773	847	21			

- Molecule 2 is a protein called GLYCEROL DEHYDRATASE REACTIVASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			815	504	149	160	2			
2	D	113	Total	C	N	O	S	0	0	0
			815	504	149	160	2			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total	O	0	0
			255	255		
4	B	46	Total	O	0	0
			46	46		
4	C	247	Total	O	0	0
			247	247		

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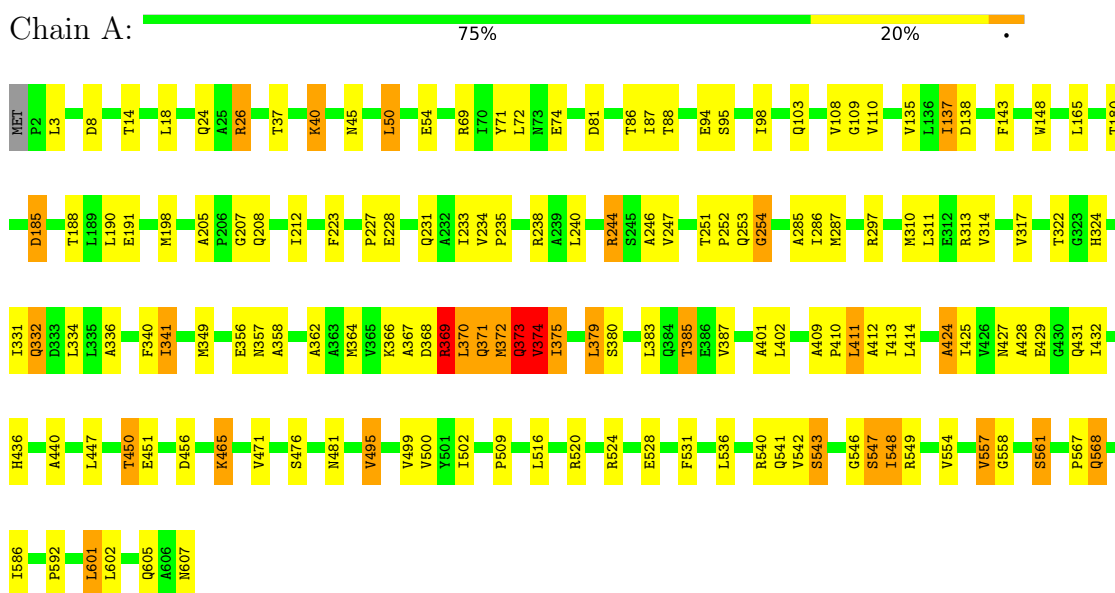
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total	O	0	0
			11	11		

3 Residue-property plots

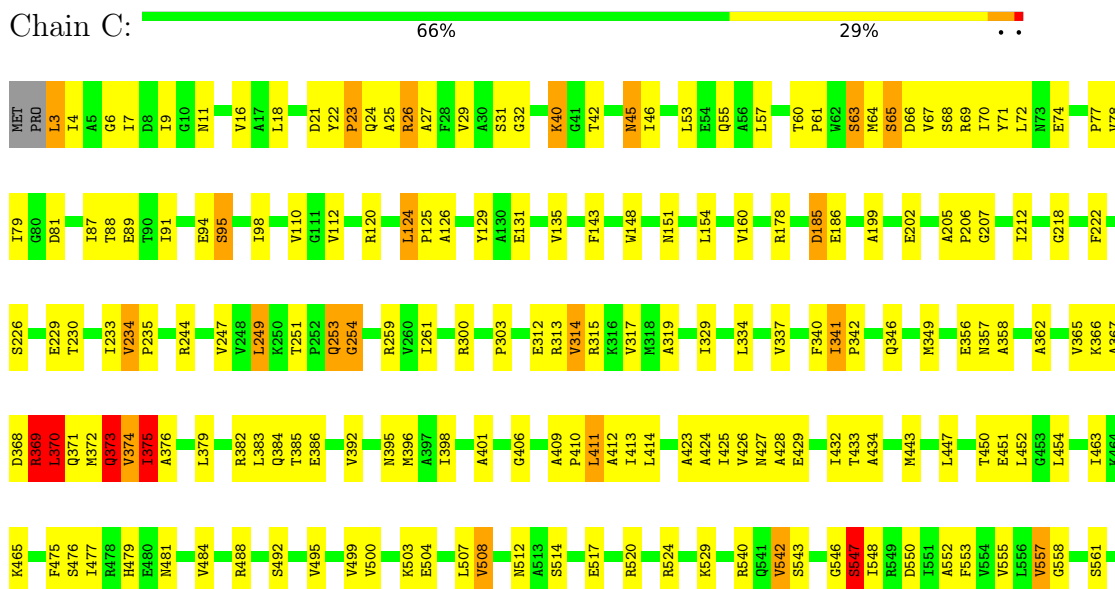
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: GLYCEROL DEHYDRATASE REACTIVASE ALPHA SUBUNIT

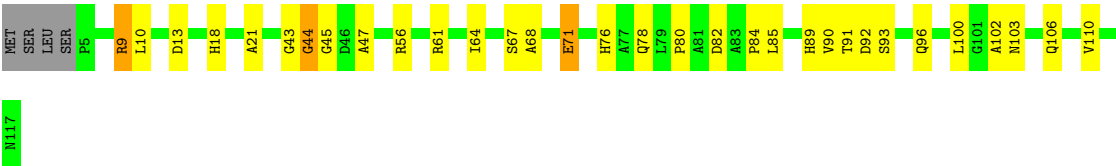




● Molecule 2: GLYCEROL DEHYDRATASE REACTIVASE BETA SUBUNIT



● Molecule 2: GLYCEROL DEHYDRATASE REACTIVASE BETA SUBUNIT



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.00Å 110.00Å 332.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11079	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: 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	0.44	0/4513	0.98	18/6135 (0.3%)
1	C	0.42	0/4496	0.98	16/6113 (0.3%)
2	B	0.40	0/831	0.90	0/1132
2	D	0.37	0/831	0.94	1/1132 (0.1%)
All	All	0.42	0/10671	0.97	35/14512 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	ARG	N-CA-C	10.29	132.71	110.80
1	A	428	ALA	N-CA-C	-8.39	102.49	112.89
1	A	369	ARG	N-CA-C	8.12	128.10	110.80
1	A	531	PHE	N-CA-C	7.37	119.39	111.36
2	D	45	GLY	N-CA-C	-6.71	101.76	110.69
1	C	428	ALA	N-CA-C	-6.69	104.06	111.82
1	A	185	ASP	N-CA-C	6.56	120.11	110.59
1	A	499	VAL	N-CA-C	-6.56	98.94	108.71
1	A	424	ALA	N-CA-C	-6.37	99.01	109.40
1	A	72	LEU	N-CA-C	6.37	119.32	109.07
1	A	137	ILE	N-CA-C	6.21	116.80	107.80
1	A	87	ILE	N-CA-C	6.17	118.03	112.17
1	C	124	LEU	N-CA-C	6.15	117.14	109.57
1	C	424	ALA	N-CA-C	-5.99	98.64	108.76
1	C	186	GLU	N-CA-C	5.94	119.38	111.30
1	C	87	ILE	N-CA-C	5.80	117.77	112.43
1	A	465	LYS	N-CA-C	5.74	120.40	113.17
1	A	547	SER	N-CA-C	5.62	117.41	111.28
1	A	135	VAL	N-CA-C	5.53	116.19	108.89
1	C	135	VAL	N-CA-C	5.51	116.70	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	542	VAL	N-CA-C	-5.48	107.41	112.83
1	C	185	ASP	N-CA-C	5.45	118.49	110.59
1	C	508	VAL	CA-C-N	5.43	125.19	119.76
1	C	508	VAL	C-N-CA	5.43	125.19	119.76
1	C	465	LYS	N-CA-C	5.32	119.87	113.17
1	A	450	THR	N-CA-C	5.31	116.76	110.97
1	C	499	VAL	N-CA-C	-5.24	102.08	109.21
1	C	234	VAL	CB-CA-C	-5.24	108.72	113.70
1	A	502	ILE	N-CA-C	5.23	115.11	107.37
1	A	244	ARG	N-CA-C	-5.19	107.11	113.50
1	A	476	SER	N-CA-C	5.18	117.86	109.06
1	A	103	GLN	N-CA-C	5.12	117.76	111.82
1	A	188	THR	N-CA-C	5.07	117.47	111.33
1	C	218	GLY	N-CA-C	-5.05	106.38	112.49
1	C	6	GLY	N-CA-C	-5.04	101.25	113.18

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	4452	0	4571	124	0
1	C	4436	0	4557	197	0
2	B	815	0	796	27	0
2	D	815	0	796	26	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	255	0	0	7	0
4	B	46	0	0	0	0
4	C	247	0	0	11	0
4	D	11	0	0	0	0
All	All	11079	0	10720	365	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 17.

All (365) 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:373:GLN:HG3	1:C:374:VAL:H	1.03	1.13
1:C:398:ILE:HA	1:C:413:ILE:HD11	1.38	1.03
1:C:370:LEU:HD22	1:C:370:LEU:H	1.23	1.01
1:A:26:ARG:HH11	1:A:26:ARG:HB3	1.28	0.96
1:C:373:GLN:HG3	1:C:374:VAL:N	1.75	0.95
1:A:471:VAL:HG21	1:A:495:VAL:HG13	1.47	0.94
2:B:80:PRO:HG2	2:B:83:ALA:HB3	1.50	0.92
1:C:26:ARG:HH11	1:C:26:ARG:HB3	1.37	0.88
1:A:567:PRO:HG2	1:A:568:GLN:OE1	1.74	0.87
1:C:26:ARG:HB3	1:C:26:ARG:NH1	1.90	0.86
1:C:45:ASN:ND2	1:C:375:ILE:HD11	1.92	0.83
1:A:26:ARG:HB3	1:A:26:ARG:NH1	1.93	0.82
1:C:94:GLU:HB2	1:C:253:GLN:HE22	1.44	0.82
1:C:341:ILE:HG23	1:C:450:THR:HG23	1.63	0.81
2:B:61:ARG:HD2	2:D:61:ARG:HD2	1.62	0.80
1:A:341:ILE:HG23	1:A:450:THR:HG23	1.64	0.79
1:C:373:GLN:CG	1:C:374:VAL:H	1.92	0.78
1:A:198:MET:HE2	1:A:223:PHE:HD2	1.49	0.78
1:C:78:VAL:HG22	1:C:366:LYS:HG3	1.67	0.77
1:C:45:ASN:HD21	1:C:375:ILE:HD11	1.50	0.76
1:A:540:ARG:HH21	1:A:548:ILE:HD12	1.51	0.74
1:C:95:SER:HB3	1:C:349:MET:SD	2.27	0.73
1:C:74:GLU:OE2	1:C:375:ILE:HB	1.88	0.73
1:A:207:GLY:HA2	1:C:481:ASN:ND2	2.02	0.73
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.54	0.73
1:C:370:LEU:H	1:C:370:LEU:CD2	2.00	0.72
1:A:198:MET:HE2	1:A:223:PHE:CD2	2.25	0.71
1:A:495:VAL:HG23	1:A:509:PRO:HG3	1.74	0.70
2:B:76:HIS:HD2	2:B:78:GLN:H	1.38	0.70
1:C:382:ARG:NH1	1:C:382:ARG:HB2	2.06	0.70
1:C:60:THR:HB	1:C:61:PRO:HD2	1.73	0.70
1:A:540:ARG:HH21	1:A:548:ILE:CD1	2.05	0.69
2:B:115:GLU:HG2	2:B:116:ARG:H	1.56	0.69
2:D:9:ARG:HG2	2:D:9:ARG:HH11	1.56	0.69
1:C:367:ALA:O	1:C:369:ARG:N	2.26	0.69
1:C:411:LEU:HD13	1:C:412:ALA:N	2.09	0.68
1:A:311:LEU:HD22	1:A:331:ILE:HD13	1.75	0.68
1:A:374:VAL:HG23	1:A:375:ILE:H	1.59	0.68
1:C:253:GLN:NE2	1:C:254:GLY:N	2.42	0.67
1:C:91:ILE:HD12	1:C:259:ARG:HH12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ARG:HG3	1:C:548:ILE:CG2	2.24	0.66
1:C:375:ILE:HG22	1:C:376:ALA:N	2.10	0.66
1:A:81:ASP:HB2	1:A:314:VAL:HG22	1.76	0.66
1:C:91:ILE:HD12	1:C:259:ARG:NH1	2.11	0.66
1:C:548:ILE:HD11	1:C:577:TYR:CG	2.32	0.65
1:A:137:ILE:HD12	1:A:165:LEU:CD2	2.28	0.64
1:A:50:LEU:O	1:A:54:GLU:HG2	1.97	0.64
1:A:375:ILE:O	1:A:379:LEU:HB2	1.96	0.64
1:C:373:GLN:O	1:C:374:VAL:HG23	1.98	0.64
1:C:392:VAL:HB	1:C:395:ASN:ND2	2.12	0.64
1:C:414:LEU:HD23	1:C:423:ALA:HB2	1.80	0.63
1:C:411:LEU:HD13	1:C:411:LEU:C	2.24	0.63
1:C:71:TYR:CZ	1:C:604:GLY:HA2	2.34	0.63
1:C:89:GLU:HB3	1:C:261:ILE:HD11	1.81	0.63
2:B:92:ASP:HB3	2:B:96:GLN:HE21	1.64	0.62
1:C:234:VAL:HB	1:C:235:PRO:HD3	1.79	0.62
1:C:374:VAL:HG12	1:C:375:ILE:N	2.14	0.62
1:C:81:ASP:HB2	1:C:314:VAL:HG23	1.82	0.62
1:C:341:ILE:HG23	1:C:450:THR:CG2	2.29	0.62
1:A:198:MET:HE1	1:A:223:PHE:HA	1.80	0.62
1:C:411:LEU:HD22	1:C:553:PHE:O	1.99	0.62
1:A:536:LEU:HD22	1:A:548:ILE:HD13	1.82	0.62
1:C:341:ILE:HD12	1:C:356:GLU:O	2.00	0.62
1:C:411:LEU:HD21	1:C:555:VAL:HG23	1.82	0.62
1:C:337:VAL:HG21	1:C:447:LEU:HD11	1.82	0.61
1:A:341:ILE:HG23	1:A:450:THR:CG2	2.30	0.61
2:D:85:LEU:C	2:D:85:LEU:HD23	2.25	0.61
1:A:367:ALA:O	1:A:369:ARG:N	2.34	0.61
1:C:253:GLN:CD	1:C:253:GLN:H	2.08	0.61
1:C:27:ALA:HB1	4:C:792:HOH:O	1.99	0.61
1:C:251:THR:OG1	1:C:254:GLY:HA3	2.00	0.61
1:C:46:ILE:HG12	1:C:375:ILE:HD13	1.82	0.61
1:A:495:VAL:HG22	1:A:500:VAL:HG11	1.82	0.60
1:C:23:PRO:O	1:C:25:ALA:N	2.34	0.60
1:A:380:SER:HB3	1:A:387:VAL:HG23	1.83	0.60
1:A:287:MET:HE3	1:A:336:ALA:HB3	1.84	0.60
2:B:89:HIS:CE1	2:B:91:THR:HG23	2.37	0.60
1:C:91:ILE:CD1	1:C:259:ARG:HH12	2.15	0.59
1:A:541:GLN:O	1:A:541:GLN:HG2	2.02	0.59
1:C:199:ALA:HB2	1:C:249:LEU:HD13	1.85	0.59
1:C:529:LYS:HD2	4:C:760:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:HD22	1:A:431:GLN:HB3	1.67	0.59
1:C:45:ASN:HD21	1:C:375:ILE:CD1	2.15	0.59
1:C:3:LEU:O	1:C:4:ILE:HD13	2.03	0.59
1:C:488:ARG:HG2	1:C:488:ARG:HH11	1.68	0.59
1:A:481:ASN:HB3	4:A:806:HOH:O	2.03	0.59
2:D:21:ALA:HB2	2:D:90:VAL:HG23	1.85	0.59
1:A:69:ARG:HD2	1:A:71:TYR:OH	2.03	0.58
1:A:568:GLN:HG3	4:A:675:HOH:O	2.04	0.58
2:D:102:ALA:O	2:D:106:GLN:HG3	2.04	0.58
1:A:401:ALA:HB2	1:A:413:ILE:HD12	1.84	0.58
1:C:492:SER:O	1:C:495:VAL:HG22	2.04	0.58
1:A:285:ALA:HB3	4:A:831:HOH:O	2.02	0.58
1:C:253:GLN:O	1:C:254:GLY:C	2.46	0.58
1:C:11:ASN:HD21	1:C:77:PRO:HA	1.69	0.57
1:C:226:SER:OG	1:C:229:GLU:HG3	2.04	0.57
1:C:411:LEU:HD22	1:C:412:ALA:H	1.69	0.57
1:A:547:SER:O	1:A:549:ARG:HG3	2.04	0.57
1:A:228:GLU:HA	1:A:231:GLN:HE21	1.69	0.57
1:C:45:ASN:HD22	1:C:45:ASN:C	2.13	0.57
1:C:65:SER:HB3	4:C:800:HOH:O	2.04	0.57
1:A:198:MET:CE	1:A:223:PHE:HA	2.35	0.56
2:D:18:HIS:CD2	2:D:90:VAL:HG11	2.40	0.56
1:A:253:GLN:O	1:A:254:GLY:C	2.47	0.56
2:B:6:PRO:HG3	1:C:475:PHE:CE2	2.40	0.56
1:C:500:VAL:HG11	1:C:507:LEU:HB3	1.87	0.56
1:C:517:GLU:CD	1:C:517:GLU:H	2.14	0.56
1:C:205:ALA:HB1	1:C:206:PRO:HD2	1.88	0.56
1:C:71:TYR:O	1:C:600:LEU:HD13	2.06	0.56
1:C:9:ILE:CD1	1:C:72:LEU:HD11	2.36	0.55
1:A:524:ARG:O	1:A:528:GLU:HG3	2.06	0.55
1:C:512:ASN:ND2	1:C:514:SER:OG	2.39	0.55
2:D:47:ALA:HB2	2:D:71:GLU:HB2	1.88	0.55
1:C:3:LEU:O	1:C:68:SER:HB3	2.07	0.55
1:C:72:LEU:HD21	1:C:375:ILE:CG2	2.37	0.55
2:B:115:GLU:O	2:B:116:ARG:HB2	2.06	0.55
1:C:373:GLN:CG	1:C:374:VAL:N	2.57	0.55
1:C:94:GLU:CB	1:C:253:GLN:HE22	2.16	0.55
1:C:375:ILE:O	1:C:379:LEU:HB2	2.07	0.54
2:B:85:LEU:HD23	2:B:85:LEU:O	2.07	0.54
2:D:67:SER:OG	2:D:71:GLU:HG3	2.08	0.54
1:C:64:MET:O	1:C:67:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.22	0.54
1:C:112:VAL:HG21	1:C:222:PHE:CD2	2.43	0.54
1:C:414:LEU:CD2	1:C:423:ALA:HB2	2.37	0.54
1:A:540:ARG:HG3	1:A:546:GLY:HA2	1.90	0.54
1:A:495:VAL:HG22	1:A:500:VAL:CG1	2.37	0.53
1:A:373:GLN:O	1:A:374:VAL:HG13	2.07	0.53
1:A:205:ALA:HB3	1:A:208:GLN:HG3	1.90	0.53
1:A:233:ILE:C	1:A:233:ILE:HD12	2.33	0.53
2:D:9:ARG:HG2	2:D:9:ARG:NH1	2.22	0.53
1:A:411:LEU:C	1:A:411:LEU:HD23	2.32	0.53
1:A:287:MET:HE3	1:A:336:ALA:CB	2.38	0.53
1:A:542:VAL:O	1:A:543:SER:HB3	2.09	0.53
1:A:369:ARG:CZ	1:A:371:GLN:O	2.56	0.53
1:A:547:SER:O	1:A:549:ARG:N	2.33	0.53
1:C:131:GLU:HG3	4:C:733:HOH:O	2.08	0.53
1:A:341:ILE:CD1	1:A:356:GLU:HB2	2.39	0.52
1:C:300:ARG:HG3	1:C:300:ARG:HH11	1.75	0.52
1:A:286:ILE:HG22	1:A:287:MET:HE2	1.92	0.52
1:A:313:ARG:O	1:A:317:VAL:HG23	2.10	0.52
2:B:13:ASP:OD1	2:B:15:ARG:HD2	2.10	0.52
2:D:89:HIS:CE1	2:D:91:THR:HG23	2.44	0.52
2:B:21:ALA:HB2	2:B:90:VAL:HG13	1.90	0.52
1:C:88:THR:HG21	1:C:357:ASN:HD22	1.74	0.52
1:A:137:ILE:HB	1:A:165:LEU:HD22	1.92	0.52
1:A:369:ARG:O	1:A:370:LEU:HB2	2.09	0.52
1:A:414:LEU:HD12	1:A:414:LEU:N	2.24	0.52
1:C:548:ILE:HD11	1:C:577:TYR:CD1	2.44	0.52
1:C:374:VAL:O	1:C:375:ILE:C	2.53	0.52
1:C:477:ILE:O	1:C:477:ILE:HG13	2.08	0.52
2:D:103:ASN:HA	2:D:106:GLN:OE1	2.10	0.52
1:A:332:GLN:HE22	1:A:366:LYS:H	1.57	0.51
1:A:380:SER:HB3	1:A:387:VAL:CG2	2.40	0.51
1:A:310:MET:O	1:A:314:VAL:HG23	2.10	0.51
1:C:79:ILE:HD13	1:C:317:VAL:HG12	1.92	0.51
1:A:26:ARG:HH11	1:A:26:ARG:CB	2.13	0.51
1:A:240:LEU:HD13	1:A:246:ALA:HB1	1.92	0.51
2:B:35:PRO:HG3	1:C:488:ARG:NH1	2.25	0.51
1:C:46:ILE:HG12	1:C:375:ILE:CD1	2.40	0.51
1:A:379:LEU:HD22	1:A:383:LEU:HD12	1.93	0.51
1:C:557:VAL:HG13	1:C:558:GLY:N	2.25	0.51
1:A:86:THR:HG23	1:A:341:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:OE1	1:A:253:GLN:HA	2.11	0.51
1:A:369:ARG:HG2	1:A:371:GLN:HB2	1.93	0.51
2:B:115:GLU:HG2	2:B:116:ARG:N	2.23	0.51
1:C:476:SER:HB3	4:C:877:HOH:O	2.10	0.51
1:A:557:VAL:HG13	1:A:558:GLY:N	2.26	0.51
2:D:56:ARG:HG2	2:D:56:ARG:HH11	1.75	0.51
1:C:341:ILE:CG1	1:C:358:ALA:HB2	2.41	0.50
1:C:154:LEU:HD21	1:C:160:VAL:HB	1.93	0.50
1:C:382:ARG:HB2	1:C:382:ARG:HH11	1.74	0.50
1:C:341:ILE:HD11	1:C:358:ALA:HB2	1.94	0.50
2:B:106:GLN:OE1	2:B:113:LEU:HA	2.11	0.50
1:A:234:VAL:HG21	1:C:580:VAL:HG22	1.93	0.50
1:A:409:ALA:HA	1:A:410:PRO:C	2.37	0.50
1:C:126:ALA:HA	1:C:129:TYR:CE1	2.47	0.50
1:A:40:LYS:HA	1:A:45:ASN:OD1	2.12	0.49
1:C:126:ALA:HA	1:C:129:TYR:CD1	2.47	0.49
1:A:369:ARG:HG2	1:A:371:GLN:CB	2.42	0.49
2:B:80:PRO:HG2	2:B:83:ALA:CB	2.32	0.49
1:A:137:ILE:HD12	1:A:165:LEU:HD22	1.92	0.49
1:A:425:ILE:O	1:A:432:ILE:HA	2.12	0.49
1:C:547:SER:HB3	1:C:550:ASP:OD2	2.13	0.49
1:A:322:THR:O	1:A:324:HIS:ND1	2.46	0.49
2:B:114:SER:O	2:B:115:GLU:O	2.30	0.49
1:A:86:THR:HG23	1:A:341:ILE:CD1	2.43	0.49
1:C:566:ILE:HB	1:C:567:PRO:HD3	1.95	0.49
1:A:180:THR:HG22	4:A:741:HOH:O	2.12	0.49
1:C:94:GLU:HG3	1:C:253:GLN:OE1	2.13	0.49
1:A:74:GLU:OE1	1:A:375:ILE:HD12	2.13	0.48
1:C:341:ILE:HD12	1:C:341:ILE:H	1.78	0.48
1:C:500:VAL:HG13	1:C:508:VAL:N	2.27	0.48
1:C:520:ARG:O	1:C:524:ARG:HG3	2.12	0.48
1:C:425:ILE:O	1:C:432:ILE:HA	2.13	0.48
1:C:524:ARG:HD3	4:C:825:HOH:O	2.13	0.48
1:A:366:LYS:HB3	4:A:897:HOH:O	2.13	0.48
1:C:337:VAL:HG22	1:C:443:MET:HE2	1.94	0.48
1:A:3:LEU:HD11	1:A:18:LEU:HG	1.96	0.48
1:A:234:VAL:CG2	1:C:580:VAL:HG22	2.43	0.48
1:A:414:LEU:HD13	1:A:554:VAL:HG13	1.95	0.48
1:A:586:ILE:HD12	1:A:586:ILE:N	2.29	0.48
1:C:3:LEU:HD22	1:C:18:LEU:HD11	1.95	0.48
1:A:334:LEU:C	1:A:334:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:HB2	1:C:605:GLN:HE21	1.78	0.48
1:A:238:ARG:HG3	1:C:572:GLU:OE1	2.14	0.48
1:A:425:ILE:HD13	1:A:542:VAL:HG11	1.96	0.48
1:A:98:ILE:HB	1:A:247:VAL:HB	1.94	0.47
1:A:341:ILE:HG13	1:A:358:ALA:HB2	1.96	0.47
1:A:601:LEU:O	1:A:605:GLN:HG3	2.14	0.47
1:C:40:LYS:HB3	1:C:40:LYS:NZ	2.29	0.47
1:C:382:ARG:HH11	1:C:382:ARG:CB	2.28	0.47
2:D:82:ASP:C	2:D:84:PRO:HD3	2.40	0.47
1:A:244:ARG:O	1:A:244:ARG:HG2	2.15	0.47
1:A:364:MET:HE2	1:A:436:HIS:O	2.15	0.47
1:C:95:SER:HB3	1:C:349:MET:CE	2.44	0.47
1:A:95:SER:HB3	1:A:349:MET:SD	2.54	0.47
1:A:427:ASN:HB3	1:A:429:GLU:H	1.79	0.47
2:D:93:SER:OG	2:D:96:GLN:HG3	2.15	0.47
1:A:542:VAL:O	1:A:543:SER:CB	2.62	0.47
2:B:43:GLY:O	2:B:44:GLY:O	2.32	0.47
1:C:319:ALA:HB2	1:C:329:ILE:HG13	1.96	0.47
2:D:13:ASP:OD1	2:D:68:ALA:HB2	2.15	0.47
1:A:108:VAL:HG22	1:A:109:GLY:N	2.30	0.47
1:A:227:PRO:HA	1:C:406:GLY:O	2.15	0.47
1:C:22:TYR:O	1:C:23:PRO:O	2.32	0.47
1:C:398:ILE:CA	1:C:413:ILE:HD11	2.28	0.47
1:C:548:ILE:HD11	1:C:577:TYR:CD2	2.49	0.46
1:A:251:THR:OG1	1:A:254:GLY:HA3	2.15	0.46
1:A:520:ARG:O	1:A:524:ARG:HG3	2.16	0.46
1:C:312:GLU:OE2	1:C:315:ARG:NH1	2.49	0.46
1:A:516:LEU:C	1:A:516:LEU:HD23	2.41	0.46
1:C:69:ARG:NH1	1:C:71:TYR:OH	2.49	0.46
1:C:98:ILE:HB	1:C:247:VAL:HB	1.97	0.46
1:C:401:ALA:CB	1:C:413:ILE:HG12	2.45	0.46
2:D:80:PRO:C	2:D:82:ASP:H	2.22	0.46
1:C:476:SER:OG	1:C:484:VAL:CG1	2.64	0.46
1:C:89:GLU:OE1	1:C:259:ARG:NH1	2.48	0.46
1:C:110:VAL:HG21	1:C:212:ILE:HD12	1.97	0.46
1:C:42:THR:O	1:C:45:ASN:ND2	2.49	0.46
1:C:124:LEU:HA	1:C:125:PRO:HD3	1.86	0.46
2:D:43:GLY:O	2:D:44:GLY:O	2.33	0.46
2:B:115:GLU:O	2:B:116:ARG:CB	2.63	0.46
1:C:11:ASN:ND2	1:C:77:PRO:HA	2.30	0.46
1:C:233:ILE:C	1:C:233:ILE:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:HIS:CE1	2:D:78:GLN:HG3	2.50	0.46
1:A:341:ILE:HD12	1:A:341:ILE:H	1.81	0.46
1:C:557:VAL:HG22	1:C:592:PRO:O	2.15	0.46
1:C:410:PRO:HG2	1:C:552:ALA:H	1.81	0.45
1:C:564:PHE:CD1	1:C:565:GLU:HG3	2.51	0.45
1:A:227:PRO:O	1:A:231:GLN:HG3	2.17	0.45
1:A:481:ASN:ND2	1:C:207:GLY:HA2	2.31	0.45
1:A:94:GLU:OE1	1:A:254:GLY:N	2.50	0.45
1:A:369:ARG:O	1:A:370:LEU:CB	2.65	0.45
1:C:374:VAL:O	1:C:376:ALA:N	2.50	0.45
2:B:76:HIS:CD2	2:B:78:GLN:H	2.25	0.45
1:C:540:ARG:HG3	1:C:548:ILE:HG23	1.97	0.45
1:C:45:ASN:ND2	1:C:45:ASN:C	2.75	0.45
1:C:365:VAL:HG13	1:C:365:VAL:O	2.16	0.45
1:C:398:ILE:HA	1:C:413:ILE:CD1	2.27	0.45
1:C:370:LEU:HD22	1:C:370:LEU:N	2.08	0.45
2:D:90:VAL:HG22	2:D:90:VAL:O	2.17	0.45
2:B:75:THR:OG1	2:B:76:HIS:N	2.50	0.44
1:C:340:PHE:O	1:C:451:GLU:HA	2.17	0.44
1:A:341:ILE:CG1	1:A:358:ALA:HB2	2.48	0.44
1:C:16:VAL:O	1:C:31:SER:HA	2.17	0.44
1:C:143:PHE:CD1	1:C:143:PHE:C	2.95	0.44
1:C:500:VAL:HG13	1:C:508:VAL:H	1.83	0.44
1:A:8:ASP:O	1:A:14:THR:HA	2.17	0.44
1:C:94:GLU:CG	1:C:253:GLN:NE2	2.81	0.44
1:C:373:GLN:O	1:C:374:VAL:CG2	2.65	0.44
1:A:411:LEU:HD23	1:A:412:ALA:N	2.33	0.44
1:A:110:VAL:HG21	1:A:212:ILE:HD12	1.98	0.44
1:A:191:GLU:H	1:A:191:GLU:CD	2.26	0.44
1:A:369:ARG:NE	1:A:371:GLN:O	2.51	0.44
1:C:341:ILE:HG13	1:C:358:ALA:HB2	1.99	0.44
1:C:346:GLN:HB2	4:C:715:HOH:O	2.17	0.44
2:B:115:GLU:CG	2:B:116:ARG:N	2.81	0.44
1:C:384:GLN:HA	1:C:384:GLN:OE1	2.18	0.44
1:C:542:VAL:HG12	1:C:542:VAL:O	2.17	0.44
1:A:143:PHE:CD1	1:A:143:PHE:C	2.96	0.44
1:A:148:TRP:CD1	1:A:148:TRP:C	2.96	0.44
1:C:433:THR:HG22	1:C:434:ALA:N	2.31	0.44
1:C:7:ILE:HD12	1:C:70:ILE:CG2	2.48	0.43
1:C:398:ILE:HD13	1:C:413:ILE:HD11	2.00	0.43
1:C:454:LEU:HD11	1:C:463:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASP:OD2	1:C:22:TYR:N	2.51	0.43
1:C:398:ILE:HD13	1:C:413:ILE:CD1	2.48	0.43
1:C:558:GLY:O	1:C:561:SER:OG	2.30	0.43
1:A:94:GLU:HB2	1:A:254:GLY:HA2	2.00	0.43
1:C:72:LEU:HD21	1:C:375:ILE:HG21	2.00	0.43
2:D:18:HIS:CD2	2:D:90:VAL:HG21	2.53	0.43
2:B:87:THR:O	2:B:116:ARG:NH2	2.49	0.43
1:C:4:ILE:HD12	1:C:69:ARG:HB2	1.99	0.43
1:A:456:ASP:HB2	4:A:896:HOH:O	2.19	0.43
1:A:88:THR:HG21	1:A:357:ASN:HD22	1.82	0.43
1:A:137:ILE:HD12	1:A:165:LEU:HD21	1.99	0.43
1:A:374:VAL:O	1:A:375:ILE:C	2.60	0.43
2:B:115:GLU:N	2:B:115:GLU:OE1	2.52	0.43
1:C:411:LEU:HD22	1:C:412:ALA:N	2.34	0.43
1:C:110:VAL:HG22	1:C:202:GLU:HG3	2.00	0.42
1:C:395:ASN:HA	1:C:432:ILE:HD13	2.01	0.42
1:C:396:MET:HE2	1:C:396:MET:HA	2.00	0.42
1:C:503:LYS:O	1:C:504:GLU:HB2	2.19	0.42
1:C:29:VAL:HB	1:C:587:ARG:NH2	2.33	0.42
1:A:557:VAL:HG22	1:A:592:PRO:O	2.19	0.42
1:C:9:ILE:HD11	1:C:72:LEU:HD11	2.01	0.42
1:C:81:ASP:CB	1:C:314:VAL:HG23	2.49	0.42
1:C:547:SER:HB3	1:C:550:ASP:CG	2.44	0.42
1:A:558:GLY:O	1:A:561:SER:HB2	2.20	0.42
1:A:137:ILE:O	1:A:190:LEU:HD22	2.19	0.42
2:B:10:LEU:C	2:B:10:LEU:HD23	2.45	0.42
1:C:18:LEU:CD2	1:C:57:LEU:HD23	2.49	0.42
2:D:110:VAL:HG12	2:D:110:VAL:O	2.18	0.42
1:C:94:GLU:HG3	1:C:253:GLN:CD	2.44	0.42
1:C:409:ALA:HA	1:C:410:PRO:C	2.44	0.42
2:D:80:PRO:C	2:D:82:ASP:N	2.78	0.42
1:A:234:VAL:N	1:A:235:PRO:CD	2.83	0.42
1:A:340:PHE:O	1:A:451:GLU:HA	2.20	0.42
1:C:342:PRO:HG2	4:C:697:HOH:O	2.19	0.42
2:B:85:LEU:HD23	2:B:85:LEU:C	2.45	0.42
2:D:89:HIS:O	2:D:92:ASP:OD1	2.38	0.42
1:A:37:THR:O	1:A:45:ASN:ND2	2.52	0.41
1:A:383:LEU:CB	1:A:385:THR:HG22	2.50	0.41
2:B:103:ASN:HB3	2:B:113:LEU:HD13	2.02	0.41
1:C:373:GLN:O	1:C:374:VAL:CB	2.68	0.41
1:C:586:ILE:HD12	1:C:586:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:HD23	1:A:411:LEU:HD13	2.02	0.41
1:C:369:ARG:O	1:C:371:GLN:N	2.54	0.41
1:C:313:ARG:HG3	1:C:313:ARG:HH11	1.84	0.41
1:C:557:VAL:HG22	1:C:592:PRO:C	2.45	0.41
1:C:148:TRP:CD1	1:C:148:TRP:C	2.97	0.41
1:C:334:LEU:HA	1:C:362:ALA:O	2.21	0.41
1:A:371:GLN:O	1:A:372:MET:HB3	2.20	0.41
1:C:32:GLY:HA2	1:C:55:GLN:OE1	2.20	0.41
1:C:373:GLN:C	1:C:374:VAL:HG23	2.44	0.41
1:A:540:ARG:NH1	4:A:708:HOH:O	2.54	0.41
1:C:151:ASN:OD1	1:C:178:ARG:HG2	2.20	0.41
1:C:334:LEU:C	1:C:334:LEU:HD23	2.45	0.41
1:C:507:LEU:CD1	1:C:507:LEU:N	2.83	0.41
1:A:334:LEU:HA	1:A:362:ALA:O	2.20	0.41
1:C:546:GLY:O	1:C:547:SER:C	2.63	0.41
2:B:13:ASP:OD1	2:B:15:ARG:HB2	2.21	0.41
1:C:45:ASN:HD21	1:C:375:ILE:CG1	2.33	0.41
1:C:53:LEU:CG	1:C:64:MET:HE1	2.51	0.41
1:C:230:THR:O	1:C:233:ILE:HG13	2.20	0.41
1:C:303:PRO:HA	4:C:874:HOH:O	2.20	0.41
1:C:426:VAL:O	1:C:426:VAL:HG13	2.21	0.41
1:C:429:GLU:N	1:C:429:GLU:OE2	2.54	0.41
1:C:479:HIS:HB3	4:C:752:HOH:O	2.20	0.41
2:D:10:LEU:HD23	2:D:10:LEU:C	2.46	0.41
2:D:71:GLU:HG3	2:D:71:GLU:H	1.72	0.41
1:C:81:ASP:HB2	1:C:314:VAL:CG2	2.48	0.40
1:C:94:GLU:O	1:C:251:THR:HG21	2.20	0.40
1:A:602:LEU:HD23	1:A:602:LEU:HA	1.97	0.40
1:C:3:LEU:C	1:C:4:ILE:HD13	2.46	0.40
1:C:21:ASP:HB2	1:C:605:GLN:NE2	2.36	0.40
1:C:57:LEU:HD13	1:C:63:SER:C	2.47	0.40
1:C:199:ALA:CB	1:C:249:LEU:HD13	2.50	0.40
1:C:300:ARG:HG3	1:C:300:ARG:NH1	2.35	0.40
1:C:385:THR:HG22	1:C:386:GLU:N	2.36	0.40
1:C:481:ASN:HB3	4:C:726:HOH:O	2.21	0.40
1:A:413:ILE:CG2	1:A:424:ALA:HB3	2.52	0.40
1:C:244:ARG:O	1:C:244:ARG:HG2	2.20	0.40
2:D:10:LEU:HG	2:D:64:ILE:HB	2.02	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	604/607 (100%)	567 (94%)	24 (4%)	13 (2%)	5	6
1	C	602/607 (99%)	566 (94%)	24 (4%)	12 (2%)	6	7
2	B	111/117 (95%)	102 (92%)	6 (5%)	3 (3%)	4	4
2	D	111/117 (95%)	104 (94%)	6 (5%)	1 (1%)	14	22
All	All	1428/1448 (99%)	1339 (94%)	60 (4%)	29 (2%)	6	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	MET
1	A	373	GLN
1	A	374	VAL
1	A	543	SER
2	B	44	GLY
2	B	115	GLU
2	B	116	ARG
1	C	23	PRO
1	C	24	GLN
1	C	368	ASP
1	C	369	ARG
1	C	370	LEU
1	C	372	MET
1	C	374	VAL
1	C	375	ILE
1	C	547	SER
1	A	24	GLN
1	A	368	ASP
1	A	375	ILE
1	C	254	GLY
2	D	44	GLY
1	A	369	ARG

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Mol	Chain	Res	Type
1	A	370	LEU
1	C	373	GLN
1	A	254	GLY
1	A	440	ALA
1	A	548	ILE
1	A	252	PRO
1	C	543	SER

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	461/462 (100%)	439 (95%)	22 (5%)	23	40
1	C	459/462 (99%)	437 (95%)	22 (5%)	23	40
2	B	82/86 (95%)	80 (98%)	2 (2%)	43	65
2	D	82/86 (95%)	79 (96%)	3 (4%)	30	51
All	All	1084/1096 (99%)	1035 (96%)	49 (4%)	24	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	40	LYS
1	A	50	LEU
1	A	138	ASP
1	A	185	ASP
1	A	297	ARG
1	A	332	GLN
1	A	341	ILE
1	A	371	GLN
1	A	373	GLN
1	A	374	VAL
1	A	379	LEU
1	A	385	THR
1	A	411	LEU

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Mol	Chain	Res	Type
1	A	447	LEU
1	A	465	LYS
1	A	495	VAL
1	A	557	VAL
1	A	561	SER
1	A	568	GLN
1	A	601	LEU
1	A	607	ASN
2	B	66	LEU
2	B	115	GLU
1	C	3	LEU
1	C	26	ARG
1	C	40	LYS
1	C	45	ASN
1	C	63	SER
1	C	65	SER
1	C	66	ASP
1	C	95	SER
1	C	185	ASP
1	C	249	LEU
1	C	253	GLN
1	C	314	VAL
1	C	341	ILE
1	C	370	LEU
1	C	373	GLN
1	C	375	ILE
1	C	383	LEU
1	C	411	LEU
1	C	427	ASN
1	C	452	LEU
1	C	547	SER
1	C	557	VAL
2	D	9	ARG
2	D	71	GLU
2	D	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	257	GLN
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	357	ASN
1	A	373	GLN
1	A	427	ASN
1	A	525	GLN
1	A	607	ASN
2	B	76	HIS
2	B	78	GLN
2	B	96	GLN
2	B	117	ASN
1	C	11	ASN
1	C	45	ASN
1	C	128	GLN
1	C	159	ASN
1	C	243	ASN
1	C	253	GLN
1	C	357	ASN
1	C	371	GLN
1	C	373	GLN
1	C	395	ASN
1	C	427	ASN
1	C	512	ASN
1	C	525	GLN
1	C	594	ASN
1	C	605	GLN
2	D	17	HIS
2	D	18	HIS
2	D	32	GLN
2	D	78	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

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 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.