



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:52 pm BST

PDB ID : 2GSE
Title : Crystal Structure of Human Dihydropyrimidinease-like 2
Authors : Ogg, D.; Stenmark, P.; Arrowsmith, C.; Berglund, H.; Collins, R.; Edwards, A.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Hallberg, B.M.; Hammarstrom, M.; Kotenyova, T.; Kursula, P.; Nilsson-Ehle, P.; Nyman, T.; Persson, C.; Sagemark, J.; Sundstrom, M.; Holmberg-Schiavone, L.; Thorsell, A.G.; Uppenberg, J.; Van Den Berg, S.; Weigelt, J.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on : 2006-04-26
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

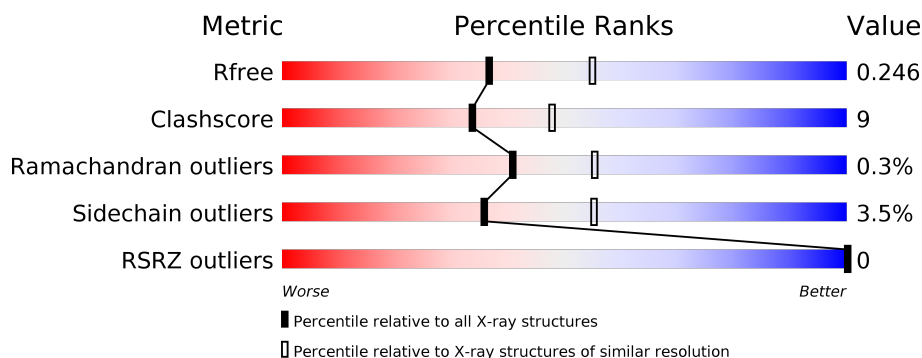
1 Overall quality at a glance

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))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	501	 75% 19% • 5%
1	B	501	 78% 15% • 5%
1	C	501	 76% 17% • 5%
1	D	501	 76% 17% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15491 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 Dihydropyrimidinase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3657	2304	625	710	18			
1	B	475	Total	C	N	O	S	0	0	0
			3657	2304	625	710	18			
1	C	475	Total	C	N	O	S	0	0	0
			3657	2304	625	710	18			
1	D	476	Total	C	N	O	S	0	0	0
			3667	2309	626	714	18			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q16555
A	-9	HIS	-	EXPRESSION TAG	UNP Q16555
A	-8	HIS	-	EXPRESSION TAG	UNP Q16555
A	-7	HIS	-	EXPRESSION TAG	UNP Q16555
A	-6	HIS	-	EXPRESSION TAG	UNP Q16555
A	-5	HIS	-	EXPRESSION TAG	UNP Q16555
A	-4	HIS	-	EXPRESSION TAG	UNP Q16555
A	-3	SER	-	CLONING ARTIFACT	UNP Q16555
A	-2	SER	-	CLONING ARTIFACT	UNP Q16555
A	-1	GLY	-	CLONING ARTIFACT	UNP Q16555
A	0	VAL	-	CLONING ARTIFACT	UNP Q16555
A	1	ASP	-	CLONING ARTIFACT	UNP Q16555
A	2	LEU	-	CLONING ARTIFACT	UNP Q16555
A	3	GLY	-	CLONING ARTIFACT	UNP Q16555
A	4	THR	-	CLONING ARTIFACT	UNP Q16555
A	5	GLU	-	CLONING ARTIFACT	UNP Q16555
A	6	ASN	-	CLONING ARTIFACT	UNP Q16555
A	7	LEU	-	CLONING ARTIFACT	UNP Q16555
A	8	TYR	-	CLONING ARTIFACT	UNP Q16555
A	9	PHE	-	CLONING ARTIFACT	UNP Q16555
A	10	GLN	-	CLONING ARTIFACT	UNP Q16555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	SER	-	CLONING ARTIFACT	UNP Q16555
A	12	MET	-	CLONING ARTIFACT	UNP Q16555
B	-10	MET	-	EXPRESSION TAG	UNP Q16555
B	-9	HIS	-	EXPRESSION TAG	UNP Q16555
B	-8	HIS	-	EXPRESSION TAG	UNP Q16555
B	-7	HIS	-	EXPRESSION TAG	UNP Q16555
B	-6	HIS	-	EXPRESSION TAG	UNP Q16555
B	-5	HIS	-	EXPRESSION TAG	UNP Q16555
B	-4	HIS	-	EXPRESSION TAG	UNP Q16555
B	-3	SER	-	CLONING ARTIFACT	UNP Q16555
B	-2	SER	-	CLONING ARTIFACT	UNP Q16555
B	-1	GLY	-	CLONING ARTIFACT	UNP Q16555
B	0	VAL	-	CLONING ARTIFACT	UNP Q16555
B	1	ASP	-	CLONING ARTIFACT	UNP Q16555
B	2	LEU	-	CLONING ARTIFACT	UNP Q16555
B	3	GLY	-	CLONING ARTIFACT	UNP Q16555
B	4	THR	-	CLONING ARTIFACT	UNP Q16555
B	5	GLU	-	CLONING ARTIFACT	UNP Q16555
B	6	ASN	-	CLONING ARTIFACT	UNP Q16555
B	7	LEU	-	CLONING ARTIFACT	UNP Q16555
B	8	TYR	-	CLONING ARTIFACT	UNP Q16555
B	9	PHE	-	CLONING ARTIFACT	UNP Q16555
B	10	GLN	-	CLONING ARTIFACT	UNP Q16555
B	11	SER	-	CLONING ARTIFACT	UNP Q16555
B	12	MET	-	CLONING ARTIFACT	UNP Q16555
C	-10	MET	-	EXPRESSION TAG	UNP Q16555
C	-9	HIS	-	EXPRESSION TAG	UNP Q16555
C	-8	HIS	-	EXPRESSION TAG	UNP Q16555
C	-7	HIS	-	EXPRESSION TAG	UNP Q16555
C	-6	HIS	-	EXPRESSION TAG	UNP Q16555
C	-5	HIS	-	EXPRESSION TAG	UNP Q16555
C	-4	HIS	-	EXPRESSION TAG	UNP Q16555
C	-3	SER	-	CLONING ARTIFACT	UNP Q16555
C	-2	SER	-	CLONING ARTIFACT	UNP Q16555
C	-1	GLY	-	CLONING ARTIFACT	UNP Q16555
C	0	VAL	-	CLONING ARTIFACT	UNP Q16555
C	1	ASP	-	CLONING ARTIFACT	UNP Q16555
C	2	LEU	-	CLONING ARTIFACT	UNP Q16555
C	3	GLY	-	CLONING ARTIFACT	UNP Q16555
C	4	THR	-	CLONING ARTIFACT	UNP Q16555
C	5	GLU	-	CLONING ARTIFACT	UNP Q16555
C	6	ASN	-	CLONING ARTIFACT	UNP Q16555

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	LEU	-	CLONING ARTIFACT	UNP Q16555
C	8	TYR	-	CLONING ARTIFACT	UNP Q16555
C	9	PHE	-	CLONING ARTIFACT	UNP Q16555
C	10	GLN	-	CLONING ARTIFACT	UNP Q16555
C	11	SER	-	CLONING ARTIFACT	UNP Q16555
C	12	MET	-	CLONING ARTIFACT	UNP Q16555
D	-10	MET	-	EXPRESSION TAG	UNP Q16555
D	-9	HIS	-	EXPRESSION TAG	UNP Q16555
D	-8	HIS	-	EXPRESSION TAG	UNP Q16555
D	-7	HIS	-	EXPRESSION TAG	UNP Q16555
D	-6	HIS	-	EXPRESSION TAG	UNP Q16555
D	-5	HIS	-	EXPRESSION TAG	UNP Q16555
D	-4	HIS	-	EXPRESSION TAG	UNP Q16555
D	-3	SER	-	CLONING ARTIFACT	UNP Q16555
D	-2	SER	-	CLONING ARTIFACT	UNP Q16555
D	-1	GLY	-	CLONING ARTIFACT	UNP Q16555
D	0	VAL	-	CLONING ARTIFACT	UNP Q16555
D	1	ASP	-	CLONING ARTIFACT	UNP Q16555
D	2	LEU	-	CLONING ARTIFACT	UNP Q16555
D	3	GLY	-	CLONING ARTIFACT	UNP Q16555
D	4	THR	-	CLONING ARTIFACT	UNP Q16555
D	5	GLU	-	CLONING ARTIFACT	UNP Q16555
D	6	ASN	-	CLONING ARTIFACT	UNP Q16555
D	7	LEU	-	CLONING ARTIFACT	UNP Q16555
D	8	TYR	-	CLONING ARTIFACT	UNP Q16555
D	9	PHE	-	CLONING ARTIFACT	UNP Q16555
D	10	GLN	-	CLONING ARTIFACT	UNP Q16555
D	11	SER	-	CLONING ARTIFACT	UNP Q16555
D	12	MET	-	CLONING ARTIFACT	UNP Q16555

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

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

- Molecule 3 is water.

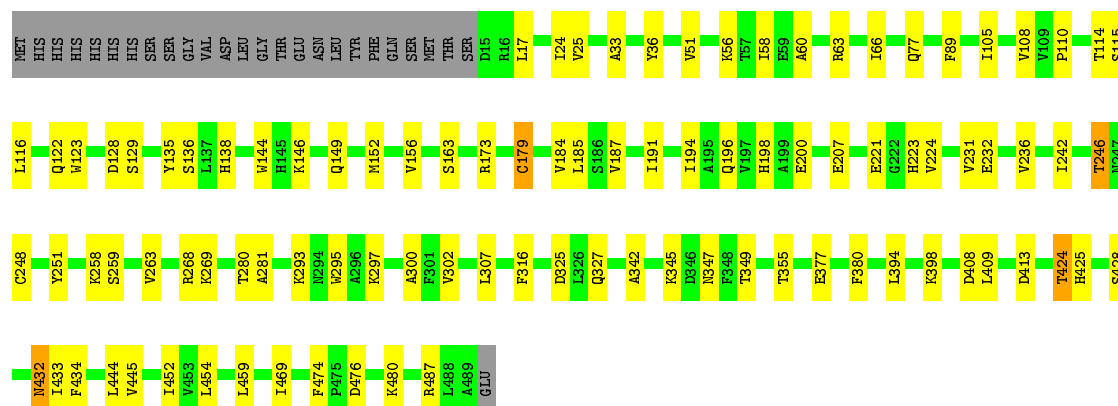
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	220	Total 220	O 220	0	0
3	B	188	Total 188	O 188	0	0
3	C	223	Total 223	O 223	0	0
3	D	218	Total 218	O 218	0	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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 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.

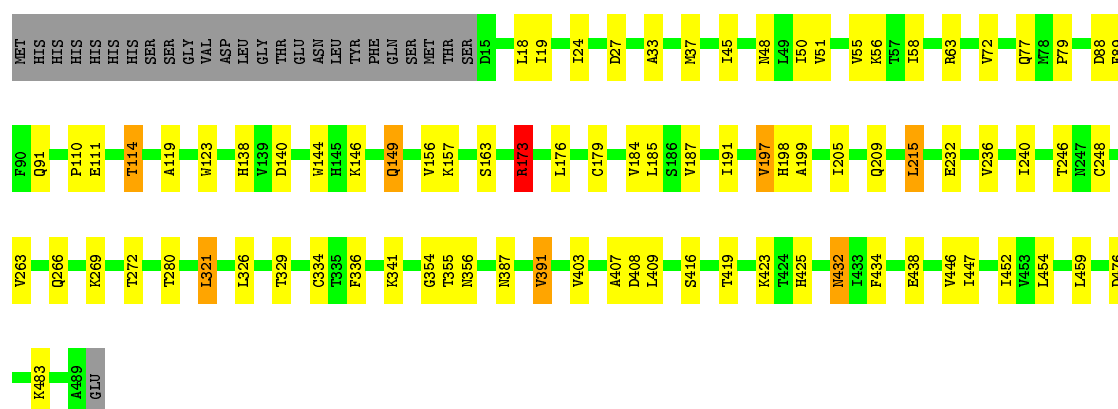
• Molecule 1: Dihydropyrimidinase-related protein 2

Chain A: 



• Molecule 1: Dihydropyrimidinase-related protein 2

Chain B: 

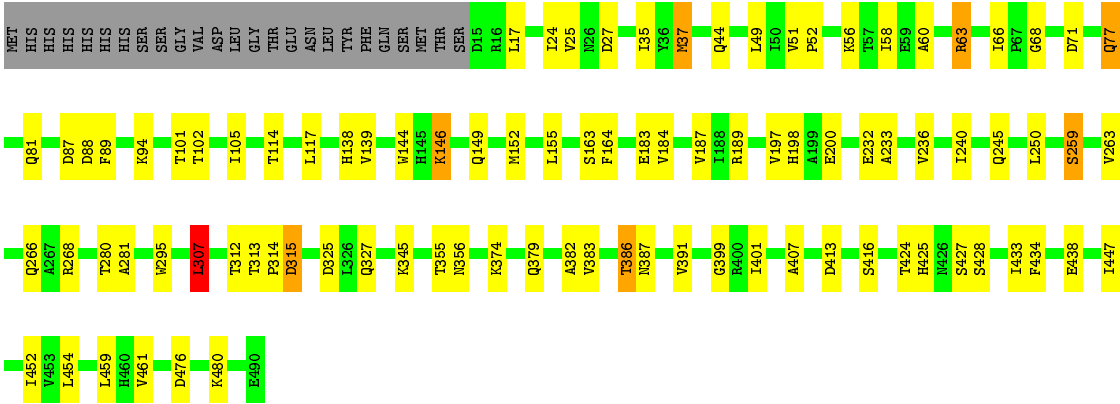


• Molecule 1: Dihydropyrimidinase-related protein 2

Chain C: 



● Molecule 1: Dihydropyrimidinase-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40 Å 126.10 Å 102.90 Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	29.31 – 2.40 29.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.31-2.40) 99.9 (29.31-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.245 0.174 , 0.246	Depositor DCC
R_{free} test set	3960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 11.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15491	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.72	1/3732 (0.0%)	0.79	2/5064 (0.0%)
1	B	0.73	1/3732 (0.0%)	0.80	4/5064 (0.1%)
1	C	0.72	1/3732 (0.0%)	0.77	1/5064 (0.0%)
1	D	0.74	0/3742	0.77	3/5076 (0.1%)
All	All	0.73	3/14938 (0.0%)	0.78	10/20268 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	179	CYS	CB-SG	-8.99	1.67	1.82
1	A	179	CYS	CB-SG	-7.18	1.70	1.82
1	B	179	CYS	CB-SG	-5.30	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	268	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	487	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	476	ASP	CB-CG-OD1	5.63	123.36	118.30
1	D	189	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	487	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	321	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	307	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	140	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	268	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3657	0	3604	59	0
1	B	3657	0	3604	62	0
1	C	3657	0	3604	61	0
1	D	3667	0	3610	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	220	0	0	8	0
3	B	188	0	0	7	0
3	C	223	0	0	6	0
3	D	218	0	0	6	0
All	All	15491	0	14422	248	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 9.

All (248) 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:37:MET:CE	1:B:407:ALA:HB1	1.86	1.05
1:B:37:MET:HE2	1:B:407:ALA:HB1	1.42	0.97
1:C:144:TRP:HZ3	1:C:152:MET:HE1	1.36	0.88
1:A:432:ASN:HD22	1:A:434:PHE:H	1.22	0.86
1:B:215:LEU:HD13	3:B:1151:HOH:O	1.78	0.83
1:A:347:ASN:OD1	1:A:349:THR:OG1	1.97	0.82
1:A:77:GLN:HE21	1:A:89:PHE:H	1.27	0.82
1:C:347:ASN:ND2	1:C:349:THR:OG1	2.13	0.81
1:D:37:MET:HE3	1:D:407:ALA:HB1	1.64	0.79
1:A:398:LYS:NZ	1:A:408:ASP:OD2	2.14	0.78
1:C:432:ASN:HD22	1:C:434:PHE:H	1.30	0.78
1:B:37:MET:HE3	1:B:407:ALA:HB1	1.62	0.78
1:D:37:MET:CE	1:D:407:ALA:HB1	2.13	0.78
1:A:149:GLN:HA	1:A:152:MET:HE2	1.64	0.77
1:D:138:HIS:HD2	1:D:163:SER:OG	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:OE1	3:A:1171:HOH:O	2.04	0.74
1:A:424:THR:HG22	3:A:1029:HOH:O	1.86	0.74
1:B:138:HIS:HD2	1:B:163:SER:OG	1.69	0.74
1:C:249:PRO:HD3	1:C:482:ILE:HD13	1.70	0.74
1:C:149:GLN:HA	1:C:152:MET:HE2	1.70	0.73
1:A:185:LEU:HB3	1:A:246:THR:HG21	1.69	0.73
1:D:37:MET:HE2	1:D:447:ILE:HG21	1.70	0.72
1:B:37:MET:HE1	1:B:447:ILE:HG21	1.70	0.72
1:B:419:THR:OG1	1:B:438:GLU:OE2	2.06	0.71
1:C:144:TRP:CZ3	1:C:152:MET:HE1	2.23	0.71
1:B:156:VAL:HG21	1:B:191:ILE:CG2	2.21	0.71
1:D:17:LEU:HD12	1:D:56:LYS:O	1.90	0.70
1:D:197:VAL:HG21	1:D:250:LEU:HD11	1.73	0.70
1:D:152:MET:HE3	1:D:187:VAL:HG11	1.73	0.69
1:B:483:LYS:HG2	3:B:1172:HOH:O	1.93	0.69
1:D:58:ILE:HD11	1:D:452:ILE:HD11	1.74	0.69
1:B:58:ILE:HD11	1:B:452:ILE:HD11	1.73	0.69
1:B:432:ASN:HD22	1:B:434:PHE:H	1.41	0.69
1:A:152:MET:CE	1:A:187:VAL:HG11	2.24	0.67
1:D:382:ALA:HA	1:D:386:THR:HG23	1.75	0.67
1:A:152:MET:HE3	1:A:187:VAL:HG11	1.78	0.66
1:A:138:HIS:HD2	1:A:163:SER:OG	1.79	0.66
1:A:58:ILE:HD11	1:A:452:ILE:HD11	1.78	0.66
1:C:464:GLY:O	3:C:1171:HOH:O	2.14	0.65
1:C:77:GLN:HE21	1:C:89:PHE:H	1.44	0.64
1:D:56:LYS:HE3	1:D:452:ILE:HD12	1.77	0.64
1:A:60:ALA:O	1:A:63:ARG:HB2	1.97	0.64
1:D:233:ALA:HB2	1:D:259:SER:HB3	1.78	0.64
1:B:355:THR:HG23	1:B:356:ASN:O	1.96	0.64
1:D:77:GLN:HE21	1:D:88:ASP:HB2	1.62	0.64
1:A:454:LEU:HD13	1:A:459:LEU:HD13	1.79	0.64
1:B:19:ILE:HD11	1:B:447:ILE:HD13	1.78	0.64
1:B:416:SER:O	3:B:1188:HOH:O	2.15	0.64
1:C:138:HIS:HD2	1:C:163:SER:OG	1.80	0.64
1:B:266:GLN:OE1	1:B:269:LYS:NZ	2.32	0.63
1:C:30:SER:O	3:C:1137:HOH:O	2.15	0.62
1:D:77:GLN:NE2	1:D:88:ASP:HB2	2.14	0.62
1:D:197:VAL:CG2	1:D:250:LEU:HD11	2.29	0.62
1:B:280:THR:HG22	1:B:434:PHE:CZ	2.34	0.62
1:D:152:MET:CE	1:D:187:VAL:HG11	2.29	0.62
1:D:266:GLN:NE2	3:D:1059:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:OD1	1:A:135:TYR:OH	2.13	0.60
1:B:321:LEU:HD12	1:B:326:LEU:O	2.01	0.59
1:B:24:ILE:HD12	1:B:33:ALA:HB3	1.84	0.59
1:D:58:ILE:HD11	1:D:452:ILE:CD1	2.31	0.59
1:D:117:LEU:HD23	1:D:155:LEU:HD21	1.84	0.59
1:D:25:VAL:HB	1:D:66:ILE:HG22	1.84	0.59
1:B:173:ARG:CG	1:B:173:ARG:HH11	2.15	0.59
1:B:37:MET:HE2	1:B:407:ALA:CB	2.26	0.59
1:B:387:ASN:O	1:B:391:VAL:HG13	2.03	0.59
1:A:280:THR:HG22	1:A:434:PHE:CZ	2.38	0.58
1:D:295:TRP:CZ2	1:D:345:LYS:HA	2.39	0.58
1:D:138:HIS:CD2	1:D:163:SER:OG	2.56	0.58
1:B:50:ILE:HG22	1:B:50:ILE:O	2.04	0.58
1:B:110:PRO:HB3	1:B:119:ALA:HB2	1.85	0.57
1:B:454:LEU:HD13	1:B:459:LEU:HD13	1.86	0.57
1:D:37:MET:CE	1:D:447:ILE:HG21	2.35	0.57
1:B:18:LEU:HD13	1:B:51:VAL:HG21	1.86	0.57
1:A:409:LEU:N	1:A:409:LEU:HD12	2.20	0.56
1:D:117:LEU:HD23	1:D:155:LEU:CD2	2.35	0.56
1:D:454:LEU:HD13	1:D:459:LEU:HD12	1.87	0.56
1:D:355:THR:HG23	1:D:356:ASN:O	2.05	0.56
1:B:205:ILE:O	1:B:209:GLN:HG3	2.06	0.56
1:B:408:ASP:C	1:B:409:LEU:HD12	2.27	0.55
1:C:148:ILE:HG22	1:C:152:MET:HE1	1.87	0.55
1:D:281:ALA:HB1	1:D:307:LEU:HD11	1.88	0.55
1:D:27:ASP:HB3	1:D:386:THR:HG21	1.89	0.55
1:C:278:PRO:HG3	1:C:326:LEU:HD13	1.88	0.55
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.42	0.54
1:C:180:GLN:O	1:C:184:VAL:HG23	2.06	0.54
3:A:1105:HOH:O	1:D:312:THR:HG21	2.05	0.54
1:C:233:ALA:HB2	1:C:259:SER:HB3	1.89	0.54
1:C:97:LEU:HD22	1:C:453:VAL:HG21	1.90	0.54
1:D:105:ILE:CG2	1:D:138:HIS:CE1	2.90	0.54
1:B:144:TRP:CE3	1:B:184:VAL:HG22	2.43	0.54
1:D:345:LYS:HB2	3:D:1060:HOH:O	2.08	0.54
1:C:432:ASN:ND2	1:C:434:PHE:H	2.02	0.53
1:B:246:THR:HG22	1:B:246:THR:O	2.06	0.53
1:C:185:LEU:HB3	1:C:246:THR:HG21	1.90	0.53
1:D:37:MET:HE1	1:D:407:ALA:HB1	1.89	0.53
1:D:355:THR:OG1	1:D:433:ILE:HG21	2.08	0.53
1:C:198:HIS:HE1	1:C:200:GLU:OE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:HG21	1:B:191:ILE:HG23	1.89	0.53
1:D:105:ILE:HG22	1:D:138:HIS:CE1	2.44	0.53
1:C:449:GLN:NE2	1:C:465:SER:O	2.40	0.53
1:C:72:VAL:O	1:C:138:HIS:HE1	1.91	0.53
1:B:111:GLU:O	1:B:114:THR:HG23	2.09	0.52
1:D:401:ILE:HD13	1:D:401:ILE:N	2.25	0.52
1:A:413:ASP:HB2	1:A:444:LEU:HG	1.91	0.52
1:C:201:ASN:H	1:C:231:VAL:HG13	1.74	0.52
1:C:52:PRO:HB2	1:C:55:VAL:HG23	1.90	0.52
1:D:149:GLN:HB2	3:D:1065:HOH:O	2.09	0.52
1:C:245:GLN:OE1	3:C:1042:HOH:O	2.19	0.52
1:A:77:GLN:NE2	1:A:89:PHE:H	2.01	0.52
1:A:77:GLN:HE21	1:A:89:PHE:N	2.04	0.51
1:B:138:HIS:CD2	1:B:163:SER:OG	2.59	0.51
1:D:245:GLN:OE1	3:D:1026:HOH:O	2.19	0.51
1:D:68:GLY:HA3	1:D:102:THR:OG1	2.11	0.51
1:A:242:ILE:O	1:A:246:THR:HB	2.11	0.51
1:C:16:ARG:CZ	1:C:52:PRO:HG2	2.41	0.51
1:C:371:VAL:HG21	1:C:440:ARG:HB3	1.94	0.50
1:A:144:TRP:CE3	1:A:184:VAL:HG22	2.46	0.50
1:A:221:GLU:O	1:A:224:VAL:HG12	2.11	0.50
1:D:81:GLN:N	3:D:1203:HOH:O	2.37	0.50
1:B:51:VAL:HG12	1:B:55:VAL:HG21	1.94	0.49
1:A:173:ARG:HD3	3:A:1073:HOH:O	2.12	0.49
1:D:386:THR:HB	1:D:399:GLY:O	2.12	0.49
1:C:148:ILE:HG22	1:C:152:MET:CE	2.42	0.49
1:B:246:THR:CG2	1:B:246:THR:O	2.60	0.49
1:A:198:HIS:HE1	1:A:200:GLU:OE1	1.94	0.49
1:A:24:ILE:HD12	1:A:33:ALA:HB3	1.95	0.49
1:C:179:CYS:O	1:C:183:GLU:HG3	2.13	0.49
1:C:481:ARG:HD3	1:D:379:GLN:HE22	1.78	0.49
1:B:232:GLU:O	1:B:236:VAL:HG23	2.12	0.48
1:D:232:GLU:O	1:D:236:VAL:HG23	2.13	0.48
1:A:232:GLU:O	1:A:236:VAL:HG23	2.13	0.48
1:A:258:LYS:HG2	1:A:316:PHE:CD2	2.49	0.48
1:B:185:LEU:HB3	1:B:246:THR:HG21	1.95	0.48
1:A:474:PHE:HE1	3:A:1046:HOH:O	1.96	0.48
1:B:72:VAL:O	1:B:138:HIS:HE1	1.97	0.48
1:B:77:GLN:NE2	1:B:88:ASP:HB2	2.29	0.47
1:B:45:ILE:HD12	1:B:403:VAL:HG23	1.96	0.47
1:B:173:ARG:HG3	1:B:173:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:CE	3:A:1206:HOH:O	2.63	0.47
1:C:227:ARG:NH2	3:C:1061:HOH:O	2.47	0.47
1:B:246:THR:HG22	1:B:248:CYS:HB2	1.97	0.47
1:C:295:TRP:CZ2	1:C:345:LYS:HA	2.50	0.47
1:D:77:GLN:HE21	1:D:89:PHE:H	1.62	0.47
1:A:432:ASN:ND2	1:A:434:PHE:H	2.02	0.47
1:A:207:GLU:HB3	1:C:182:TYR:CE1	2.49	0.47
1:B:149:GLN:HG2	1:B:187:VAL:HG21	1.96	0.47
1:C:200:GLU:OE2	1:C:227:ARG:HD3	2.14	0.47
1:A:108:VAL:HG22	1:A:123:TRP:CB	2.44	0.47
1:B:27:ASP:OD2	3:B:1159:HOH:O	2.21	0.47
1:B:446:VAL:HG23	1:B:454:LEU:HD23	1.96	0.46
1:A:105:ILE:CG2	1:A:138:HIS:CE1	2.97	0.46
1:A:293:LYS:HD2	3:A:1106:HOH:O	2.16	0.46
1:D:379:GLN:O	1:D:383:VAL:HG13	2.16	0.46
1:B:156:VAL:HG21	1:B:191:ILE:HG21	1.97	0.46
1:B:173:ARG:CG	1:B:173:ARG:NH1	2.77	0.46
1:B:77:GLN:HE21	1:B:89:PHE:H	1.64	0.46
1:C:188:ILE:HG23	1:C:193:ALA:HB3	1.98	0.46
1:A:454:LEU:CD1	1:A:459:LEU:HD13	2.44	0.46
1:C:347:ASN:C	1:C:347:ASN:HD22	2.20	0.46
1:C:77:GLN:HG2	1:C:88:ASP:CB	2.46	0.46
1:C:394:LEU:HD22	1:C:469:ILE:HG21	1.97	0.46
1:D:240:ILE:HD12	1:D:263:VAL:HG12	1.98	0.46
1:B:187:VAL:HG12	1:B:191:ILE:HD12	1.98	0.45
1:A:355:THR:OG1	1:A:433:ILE:HD13	2.15	0.45
1:A:17:LEU:HD12	1:A:56:LYS:O	2.17	0.45
1:B:197:VAL:HG13	1:B:199:ALA:HB2	1.98	0.45
1:C:446:VAL:HG23	1:C:454:LEU:HD23	1.97	0.45
1:B:334:CYS:O	1:B:354:GLY:HA3	2.16	0.45
1:D:325:ASP:O	1:D:327:GLN:NE2	2.49	0.45
1:A:295:TRP:CH2	1:A:342:ALA:HA	2.51	0.45
1:D:58:ILE:CD1	1:D:452:ILE:HD11	2.46	0.45
1:A:281:ALA:HB1	1:A:307:LEU:HD11	1.98	0.45
1:A:445:VAL:HA	1:A:454:LEU:O	2.16	0.45
1:B:157:LYS:HD2	3:B:1123:HOH:O	2.16	0.45
1:C:75:ARG:HB2	1:C:334:CYS:HB2	1.99	0.45
1:B:198:HIS:HD2	3:B:1008:HOH:O	2.00	0.45
1:D:280:THR:HG22	1:D:434:PHE:CZ	2.52	0.44
1:D:387:ASN:O	1:D:391:VAL:HG13	2.17	0.44
1:C:17:LEU:HD13	1:C:56:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLN:HB3	1:D:49:LEU:HD22	1.99	0.44
1:B:58:ILE:HD11	1:B:452:ILE:CD1	2.45	0.44
1:C:55:VAL:HG12	1:C:56:LYS:O	2.18	0.44
1:A:36:TYR:CE1	1:A:51:VAL:HG13	2.53	0.44
1:C:93:THR:HG22	1:C:104:ILE:HG12	2.00	0.44
1:A:156:VAL:HG21	1:A:191:ILE:HD12	1.98	0.44
1:C:17:LEU:HD12	1:C:18:LEU:H	1.83	0.44
1:C:200:GLU:HB3	1:C:205:ILE:HD11	1.99	0.44
1:C:73:HIS:HB2	1:C:277:GLU:OE2	2.17	0.44
1:D:146:LYS:CE	1:D:146:LYS:H	2.29	0.44
1:D:87:ASP:OD2	1:D:427:SER:OG	2.34	0.44
1:D:60:ALA:O	1:D:63:ARG:HG2	2.18	0.44
1:B:454:LEU:HD13	1:B:459:LEU:CD1	2.48	0.44
1:C:281:ALA:HB1	1:C:307:LEU:HD11	1.99	0.44
1:A:246:THR:CG2	1:A:248:CYS:HB2	2.47	0.43
1:C:356:ASN:HD21	1:C:432:ASN:ND2	2.16	0.43
1:D:94:LYS:HG3	1:D:461:VAL:HG21	1.98	0.43
1:C:16:ARG:HD3	1:C:55:VAL:HG22	2.00	0.43
1:D:413:ASP:OD2	1:D:416:SER:HB3	2.19	0.43
1:A:293:LYS:NZ	3:A:1206:HOH:O	2.44	0.43
1:A:408:ASP:C	1:A:409:LEU:HD12	2.39	0.43
1:C:219:GLY:HA3	3:C:1028:HOH:O	2.18	0.43
1:C:106:ASP:HB3	1:C:137:LEU:HD23	2.01	0.43
1:D:149:GLN:CB	3:D:1065:HOH:O	2.67	0.42
1:A:476:ASP:HB3	1:A:480:LYS:HD2	2.01	0.42
1:D:476:ASP:CG	1:D:480:LYS:HE3	2.40	0.42
1:B:240:ILE:HG23	1:B:272:THR:HG21	2.00	0.42
1:C:60:ALA:O	1:C:63:ARG:HB2	2.18	0.42
1:A:196:GLN:HA	1:A:251:TYR:HB3	2.02	0.42
1:B:263:VAL:HG23	3:B:1035:HOH:O	2.20	0.42
1:D:313:THR:HB	1:D:314:PRO:HD3	2.01	0.42
1:A:259:SER:O	1:A:263:VAL:HG23	2.20	0.42
1:B:72:VAL:HG22	1:B:329:THR:O	2.20	0.42
1:C:77:GLN:HG2	1:C:88:ASP:HB2	2.02	0.42
1:D:315:ASP:OD2	1:D:374:LYS:NZ	2.42	0.42
1:A:223:HIS:CD2	1:A:302:VAL:HG13	2.55	0.42
1:B:19:ILE:HD11	1:B:447:ILE:CD1	2.47	0.42
1:C:379:GLN:O	1:C:382:ALA:HB3	2.20	0.42
1:A:297:LYS:O	1:A:300:ALA:HB3	2.20	0.41
1:B:336:PHE:HB2	1:B:341:LYS:HE2	2.01	0.41
1:C:110:PRO:HG3	1:C:116:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:O	1:A:380:PHE:HB3	2.20	0.41
1:C:295:TRP:CH2	1:C:342:ALA:HA	2.54	0.41
1:C:24:ILE:O	1:C:30:SER:HA	2.20	0.41
1:D:139:VAL:O	1:D:164:PHE:HA	2.21	0.41
1:A:108:VAL:HG22	1:A:123:TRP:HB2	2.01	0.41
1:A:25:VAL:HB	1:A:66:ILE:HG22	2.01	0.41
1:D:144:TRP:NE1	1:D:183:GLU:OE1	2.51	0.41
1:A:110:PRO:HG3	1:A:116:LEU:HD22	2.01	0.41
1:A:327:GLN:OE1	1:A:327:GLN:N	2.54	0.41
1:D:139:VAL:HG21	1:D:155:LEU:HD13	2.03	0.41
1:D:24:ILE:HD11	1:D:35:ILE:HG12	2.01	0.41
1:B:37:MET:HE3	1:B:409:LEU:HD13	2.03	0.41
1:D:71:ASP:HB2	1:D:101:THR:HG21	2.03	0.41
1:A:394:LEU:CD2	1:A:469:ILE:HG21	2.51	0.41
1:C:304:SER:HA	1:C:305:PRO:C	2.41	0.41
1:C:139:VAL:O	1:C:164:PHE:HA	2.21	0.40
1:C:198:HIS:CE1	1:C:200:GLU:OE1	2.73	0.40
1:C:77:GLN:NE2	1:C:88:ASP:HB2	2.36	0.40
1:B:55:VAL:O	1:B:56:LYS:C	2.60	0.40
1:C:137:LEU:O	1:C:471:ARG:NH2	2.54	0.40
1:A:325:ASP:O	1:A:327:GLN:NE2	2.54	0.40
1:C:227:ARG:NH2	3:C:1211:HOH:O	2.54	0.40
1:D:144:TRP:CE3	1:D:184:VAL:HG22	2.57	0.40
1:B:77:GLN:O	1:B:79:PRO:HD3	2.22	0.40
1:D:197:VAL:CG2	1:D:250:LEU:CD1	2.98	0.40
1:D:94:LYS:HG2	1:D:459:LEU:HD23	2.03	0.40
1:D:198:HIS:HE1	1:D:200:GLU:OE1	2.04	0.40
1:D:27:ASP:HB3	1:D:386:THR:CG2	2.51	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	473/501 (94%)	448 (95%)	25 (5%)	0	100	100
1	B	473/501 (94%)	450 (95%)	21 (4%)	2 (0%)	34	48
1	C	473/501 (94%)	454 (96%)	18 (4%)	1 (0%)	47	62
1	D	474/501 (95%)	449 (95%)	23 (5%)	2 (0%)	34	48
All	All	1893/2004 (94%)	1801 (95%)	87 (5%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	PRO
1	D	52	PRO
1	B	48	ASN
1	D	77	GLN
1	B	215	LEU

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	398/422 (94%)	384 (96%)	14 (4%)	36	55
1	B	398/422 (94%)	385 (97%)	13 (3%)	38	57
1	C	398/422 (94%)	383 (96%)	15 (4%)	33	51
1	D	399/422 (94%)	386 (97%)	13 (3%)	38	57
All	All	1593/1688 (94%)	1538 (96%)	55 (4%)	36	55

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	115	SER
1	A	129	SER
1	A	136	SER
1	A	146	LYS
1	A	179	CYS

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Mol	Chain	Res	Type
1	A	194	ILE
1	A	231	VAL
1	A	246	THR
1	A	269	LYS
1	A	424	THR
1	A	425	HIS
1	A	428	SER
1	A	432	ASN
1	B	63	ARG
1	B	91	GLN
1	B	114	THR
1	B	123	TRP
1	B	146	LYS
1	B	149	GLN
1	B	173	ARG
1	B	176	LEU
1	B	197	VAL
1	B	391	VAL
1	B	423	LYS
1	B	425	HIS
1	B	432	ASN
1	C	63	ARG
1	C	106	ASP
1	C	123	TRP
1	C	146	LYS
1	C	165	LEU
1	C	176	LEU
1	C	227	ARG
1	C	231	VAL
1	C	269	LYS
1	C	347	ASN
1	C	355	THR
1	C	409	LEU
1	C	423	LYS
1	C	425	HIS
1	C	432	ASN
1	D	37	MET
1	D	51	VAL
1	D	63	ARG
1	D	114	THR
1	D	146	LYS
1	D	259	SER

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Mol	Chain	Res	Type
1	D	307	LEU
1	D	315	ASP
1	D	386	THR
1	D	424	THR
1	D	425	HIS
1	D	428	SER
1	D	438	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	138	HIS
1	A	159	HIS
1	A	198	HIS
1	A	209	GLN
1	A	237	ASN
1	A	426	ASN
1	A	432	ASN
1	A	449	GLN
1	B	61	HIS
1	B	77	GLN
1	B	138	HIS
1	B	198	HIS
1	B	237	ASN
1	B	426	ASN
1	B	432	ASN
1	C	61	HIS
1	C	77	GLN
1	C	138	HIS
1	C	149	GLN
1	C	198	HIS
1	C	209	GLN
1	C	237	ASN
1	C	245	GLN
1	C	347	ASN
1	C	426	ASN
1	C	432	ASN
1	D	77	GLN
1	D	138	HIS
1	D	198	HIS
1	D	210	GLN

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Mol	Chain	Res	Type
1	D	237	ASN
1	D	245	GLN
1	D	266	GLN
1	D	379	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/501 (94%)	-0.75	0 100 100	10, 21, 38, 50	0
1	B	475/501 (94%)	-0.74	0 100 100	10, 21, 39, 56	0
1	C	475/501 (94%)	-0.73	0 100 100	10, 21, 38, 56	0
1	D	476/501 (95%)	-0.76	0 100 100	9, 19, 39, 54	0
All	All	1901/2004 (94%)	-0.75	0 100 100	9, 21, 38, 56	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	1000	1/1	0.95	0.07	42,42,42,42	0
2	CA	D	1003	1/1	0.98	0.05	28,28,28,28	0
2	CA	C	1002	1/1	0.98	0.04	36,36,36,36	0
2	CA	B	1001	1/1	0.99	0.07	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.