

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 17, 2024 – 10:33 PM EST

PDB ID	:	3V93
Title	:	unliganded structure of TcrPDEC1 catalytic domain
Authors	:	Wang, H.; Kunz, S.; Chen, G.; Seebeck, T.; Wan, Y.; Robinson, H.; Martinelli,
		S.; Ke, H.
Deposited on	:	2011-12-23
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.00 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	Δ	9.45	3%		
1	A	345	83%	12%	• 5%
			4%		
1	В	345	81%	15%	•
			3%		
1	С	345	78%	18%	•
			12%		
1	D	345	67% 27%		• 6%
			6%		
1	E	345	79%	16%	• 5%



Mol	Chain	Length	Quality of chain		
1	F	345	78%	18%	••
1	G	345	81%	15%	·
1	Н	345	76%	17%	• 5%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21499 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace		
1	Δ	200	Total	С	Ν	0	S	0	0	0		
1	A	329	2553	1635	437	472	9	0	0	0		
1	В	222	Total	С	Ν	0	S	0	0	0		
1	D	ეეე	2579	1650	441	479	9	0	0	0		
1	С	222	Total	С	Ν	0	S	0	0	0		
1			U	000	2579	1650	441	479	9	0	0	0
1	Л	394	Total	С	Ν	0	S	0	0	0		
1	D	324	2525	1618	432	467	8	0	0	0		
1	F	300	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0		
1	Ľ	329	2555	1634	437	475	9	0	0	0		
1	F	224	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0		
1	I.	004	2586	1654	442	481	9	0	0	0		
1	C	224	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0		
1	I G	- 334	2586	1654	442	481	9	0	0	0		
1	Ц	308	Total	С	Ν	0	S	0	0	0		
	11	520	2545	1629	436	471	9		0	0		

• Molecule 1 is a protein called Cyclic nucleotide specific phosphodiesterase.

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	Е	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	Н	1	Total Zn 1 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	Е	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	Н	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	178	Total O 178 178	0	0
4	В	140	Total O 140 140	0	0
4	С	136	Total O 136 136	0	0
4	D	35	Total         O           35         35	0	0
4	Е	90	Total         O           90         90	0	0
4	F	168	Total O 168 168	0	0
4	G	147	Total O 147 147	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	81	Total O 81 81	0	0



# 3 Residue-property plots (i)

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 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: Cyclic nucleotide specific phosphodiesterase

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• Molecule 1: Cyclic nucleotide specific phosphodiesterase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	130.34Å 130.34Å 388.85Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	30.00 - 2.00	Depositor
Resolution (A)	49.99 - 1.97	EDS
% Data completeness	(Not available) $(30.00-2.00)$	Depositor
(in resolution range)	89.4 (49.99-1.97)	EDS
$R_{merge}$	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.91 (at 1.97 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.216 , $0.226$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.215 , $0.245$	DCC
$R_{free}$ test set	21151 reflections $(9.66\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , $48.9$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21499	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.36% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG, ZN

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	Bond lengths		angles
	Ullaili	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.36	0/2617	0.54	0/3560
1	В	0.34	0/2644	0.54	0/3599
1	С	0.34	0/2644	0.53	0/3599
1	D	0.29	0/2589	0.49	0/3522
1	Е	0.32	0/2619	0.53	0/3563
1	F	0.35	0/2651	0.55	0/3609
1	G	0.34	0/2651	0.53	0/3609
1	Н	0.32	0/2609	0.51	0/3549
All	All	0.33	0/21024	0.53	0/28610

There are no bond length outliers.

There are no bond angle outliers.

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	А	2553	0	2514	35	0
1	В	2579	0	2538	49	0
1	С	2579	0	2538	56	0
1	D	2525	0	2485	74	0
1	Е	2555	0	2509	48	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2586	0	2545	48	0
1	G	2586	0	2545	53	0
1	Н	2545	0	2503	57	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
4	А	178	0	0	2	0
4	В	140	0	0	1	0
4	С	136	0	0	2	0
4	D	35	0	0	1	0
4	Е	90	0	0	5	0
4	F	168	0	0	5	0
4	G	147	0	0	10	0
4	Н	81	0	0	1	0
All	All	21499	0	20177	406	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 10.

All (406) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:G:571:ILE:HG23	1:G:603:ARG:HH12	0.99	1.12
1:G:571:ILE:HG23	1:G:603:ARG:NH1	1.66	1.10
1:C:571:ILE:HG23	1:C:603:ARG:HH12	1.19	1.08
1:E:299:LYS:HD3	1:E:325:PRO:HB2	1.44	1.00
1:D:571:ILE:HG23	1:D:603:ARG:HH12	1.31	0.96
1:C:571:ILE:HG23	1:C:603:ARG:NH1	1.83	0.93



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:289:GLN:HB3	1:F:363:ARG:NH2	1.81	0.93
1:G:571:ILE:CG2	1:G:603:ARG:HH12	1.83	0.91
1:F:289:GLN:HB3	1:F:363:ARG:HH21	1.30	0.91
1:B:388:LYS:H	1:B:388:LYS:HD2	1.34	0.90
1:H:286:SER:HB2	1:H:427:PRO:HG2	1.54	0.89
1:B:300:SER:HB3	1:B:325:PRO:HG3	1.51	0.88
1:G:568:LYS:HG3	1:G:610:ALA:HB1	1.56	0.86
1:E:571:ILE:HG23	1:E:603:ARG:HH12	1.41	0.84
1:B:564:SER:HB3	1:C:600:ARG:HH21	1.46	0.80
1:D:586:HIS:CD2	1:D:593:GLU:HG2	2.16	0.80
1:G:488:THR:HG21	4:G:883:HOH:O	1.80	0.80
1:D:286:SER:HB2	1:D:427:PRO:HG2	1.64	0.80
1:B:393:HIS:NE2	1:F:504:THR:HG21	1.97	0.79
1:G:286:SER:HB2	1:G:427:PRO:HG2	1.65	0.78
1:F:281:ARG:HH21	1:H:463:ASN:HD22	1.32	0.78
1:D:363:ARG:HH11	1:D:363:ARG:HA	1.49	0.77
1:C:568:LYS:HG2	1:C:610:ALA:HB1	1.64	0.77
1:G:502:ASP:OD2	1:G:504:THR:HG22	1.84	0.76
1:C:603:ARG:HG3	1:C:603:ARG:HH11	1.50	0.76
1:D:571:ILE:HG23	1:D:603:ARG:NH1	2.01	0.76
1:D:310:LEU:HG	1:D:334:HIS:CD2	2.21	0.75
1:E:571:ILE:HG23	1:E:603:ARG:NH1	2.03	0.74
1:E:567:GLU:HG2	1:E:609:LYS:HG2	1.69	0.74
1:A:355:VAL:HG22	1:A:407:LEU:HD11	1.69	0.74
1:G:304:ILE:HG21	1:G:315:PHE:HE1	1.54	0.73
1:B:281:ARG:HH11	1:D:463:ASN:HD22	1.38	0.71
1:E:485:HIS:O	1:E:488:THR:HG22	1.90	0.71
1:H:428:VAL:HG11	1:H:441:LEU:HD12	1.72	0.71
1:F:300:SER:O	1:F:301:CYS:HB2	1.91	0.71
1:H:571:ILE:HG23	1:H:603:ARG:NH1	2.07	0.70
1:H:458:THR:O	1:H:461:MET:HB2	1.91	0.70
1:F:286:SER:HB2	1:F:427:PRO:HG2	1.74	0.69
1:C:569:SER:O	1:C:572:PRO:HD2	1.92	0.69
1:B:280:THR:HB	1:B:282:ARG:CZ	2.23	0.68
1:E:585:LEU:HD21	1:E:592:ILE:HD12	1.76	0.68
1:E:603:ARG:HG3	1:E:603:ARG:HH11	1.58	0.68
1:G:289:GLN:HB2	1:G:363:ARG:HH21	1.56	0.68
1:H:603:ARG:HG3	1:H:603:ARG:HH11	1.58	0.68
1:C:571:ILE:CG2	1:C:603:ARG:HH12	2.01	0.67
1:H:324:VAL:CG2	1:H:325:PRO:HD2	2.24	0.66
1:E:324:VAL:HG22	1:E:325:PRO:HD2	1.76	0.66



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:324:VAL:HG23	1:H:325:PRO:HD2	1.78	0.66
1:B:463:ASN:HD22	1:D:281:ARG:HH11	1.43	0.66
4:E:847:HOH:O	1:H:504:THR:HG21	1.96	0.66
1:H:282:ARG:HG2	1:H:282:ARG:O	1.96	0.66
1:C:571:ILE:HB	1:C:572:PRO:HD3	1.77	0.66
1:E:324:VAL:CG2	1:E:325:PRO:HD2	2.26	0.65
1:C:607:ALA:HB1	1:C:612:VAL:HB	1.79	0.65
1:C:391:MET:HA	1:C:391:MET:CE	2.26	0.65
1:G:595:PRO:HG2	4:G:832:HOH:O	1.94	0.65
1:H:288:VAL:HG11	1:H:441:LEU:HD11	1.78	0.65
1:B:463:ASN:ND2	1:D:281:ARG:HH11	1.95	0.65
1:C:320:VAL:HG12	1:C:327:VAL:HG22	1.78	0.65
1:F:447:PHE:CZ	1:F:470:LYS:HG3	2.33	0.64
1:F:300:SER:HB3	1:F:325:PRO:HG3	1.79	0.64
1:H:481:ASP:OD2	1:H:483:SER:HB3	1.97	0.64
1:C:586:HIS:CE1	1:C:593:GLU:HG2	2.33	0.63
1:D:298:PRO:HA	1:D:329:GLN:OE1	1.97	0.63
1:D:324:VAL:CG2	1:D:325:PRO:HD2	2.28	0.63
1:D:324:VAL:HG23	1:D:325:PRO:HD2	1.81	0.62
1:D:571:ILE:HB	1:D:572:PRO:HD3	1.79	0.62
1:B:300:SER:O	1:B:301:CYS:HB2	1.99	0.62
1:B:585:LEU:HD21	1:B:592:ILE:HD12	1.80	0.62
1:D:603:ARG:HG3	1:D:603:ARG:HH11	1.64	0.62
1:A:358:VAL:HG11	1:A:407:LEU:HD23	1.81	0.62
1:D:395:THR:OG1	1:D:398:GLU:HG3	2.00	0.62
1:H:492:HIS:HB2	1:H:584:LEU:HD21	1.80	0.62
1:B:281:ARG:HH11	1:D:463:ASN:ND2	1.97	0.62
1:G:363:ARG:NH2	4:G:921:HOH:O	2.26	0.61
1:E:388:LYS:HE3	1:E:392:GLU:OE2	2.01	0.61
1:B:280:THR:HG23	4:D:828:HOH:O	2.00	0.61
1:C:300:SER:O	1:C:301:CYS:HB2	2.00	0.61
1:F:516:LEU:CD2	1:F:585:LEU:HD11	2.31	0.61
1:C:300:SER:HB3	1:C:325:PRO:HG3	1.83	0.61
1:C:321:ALA:HA	1:C:327:VAL:CG2	2.31	0.60
1:G:328:LEU:HD11	1:G:407:LEU:HD12	1.83	0.60
1:B:388:LYS:O	1:B:392:GLU:HG3	2.01	0.60
1:D:424:VAL:HG12	1:D:424:VAL:O	2.00	0.60
1:D:309:ASP:OD1	1:D:309:ASP:O	2.20	0.60
1:B:388:LYS:N	1:B:389:PRO:HD2	2.16	0.60
1:C:321:ALA:HA	1:C:327:VAL:HG23	1.84	0.60
$1:\overline{\text{E:324:VAL:HG22}}$	4:E:869:HOH:O	2.02	0.60



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:484:LEU:O	1:C:488:THR:HG23	2.02	0.59
1:A:324:VAL:CG2	1:A:325:PRO:HD2	2.32	0.59
1:G:391:MET:CE	1:G:391:MET:HA	2.32	0.59
1:D:496:LEU:HD13	1:D:588:LEU:HD23	1.84	0.59
1:E:317:THR:HG21	1:E:375:ASP:HA	1.85	0.59
1:B:388:LYS:HD2	1:B:388:LYS:N	2.13	0.59
1:C:345:GLN:HE21	1:C:345:GLN:HA	1.67	0.59
1:D:308:VAL:HG22	1:D:308:VAL:O	2.02	0.59
1:F:462:ASP:HB2	4:F:889:HOH:O	2.00	0.59
1:D:354:LEU:C	1:D:354:LEU:HD23	2.23	0.59
1:D:595:PRO:O	1:D:599:LEU:HD22	2.02	0.59
1:G:603:ARG:CZ	4:G:847:HOH:O	2.50	0.59
1:A:304:ILE:HG12	1:A:334:HIS:CE1	2.37	0.58
1:A:304:ILE:H	1:A:334:HIS:HE1	1.50	0.58
1:E:463:ASN:HD22	1:G:281:ARG:HH11	1.52	0.58
1:G:289:GLN:HB2	1:G:363:ARG:NH2	2.19	0.58
1:H:310:LEU:HG	1:H:334:HIS:CD2	2.39	0.58
1:D:426:ASP:OD1	1:D:428:VAL:HG22	2.04	0.57
1:H:441:LEU:C	1:H:441:LEU:HD23	2.24	0.57
1:C:492:HIS:HB2	1:C:584:LEU:HD21	1.85	0.57
1:E:583:ASP:O	1:E:587:GLN:HG3	2.04	0.57
1:F:282:ARG:HD3	1:F:282:ARG:C	2.25	0.57
1:H:585:LEU:HD21	1:H:592:ILE:HD12	1.85	0.57
1:G:345:GLN:HA	1:G:345:GLN:NE2	2.19	0.56
1:G:282:ARG:O	1:G:282:ARG:HD3	2.06	0.56
1:D:366:PRO:HD2	1:D:541:GLU:HG2	1.88	0.56
1:F:516:LEU:HD23	1:F:585:LEU:HD11	1.86	0.56
1:D:286:SER:HB2	1:D:427:PRO:CG	2.36	0.56
1:D:317:THR:HG23	1:D:327:VAL:HG11	1.88	0.56
1:H:282:ARG:H	1:H:282:ARG:HD2	1.70	0.56
1:B:568:LYS:NZ	1:C:580:PRO:HB3	2.21	0.55
1:E:308:VAL:O	1:E:309:ASP:HB2	2.04	0.55
1:H:579:ILE:HB	1:H:580:PRO:HD3	1.88	0.55
1:G:561:GLU:HG3	4:G:894:HOH:O	2.05	0.55
1:B:281:ARG:NH1	1:D:463:ASN:HD22	2.03	0.54
1:B:447:PHE:CE1	1:B:470:LYS:HG3	2.43	0.54
1:D:309:ASP:CG	1:D:312:ASP:HB3	2.28	0.54
1:G:424:VAL:HG12	1:G:424:VAL:O	2.06	0.54
1:D:308:VAL:O	1:D:309:ASP:HB3	2.05	0.54
1:A:324:VAL:HG22	1:A:325:PRO:HD2	1.89	0.54
1:D:397:LEU:C	1:D:397:LEU:HD23	2.28	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:391:MET:HA	1:E:391:MET:CE	2.37	0.54
1:E:376:VAL:HG22	1:E:521:ASP:HA	1.89	0.54
1:B:280:THR:HG22	1:B:281:ARG:N	2.21	0.54
1:F:584:LEU:HD23	1:F:584:LEU:C	2.28	0.54
1:C:306:THR:HG22	1:C:307:ASP:N	2.23	0.54
1:D:333:MET:O	1:D:337:LEU:HG	2.08	0.54
1:C:376:VAL:HG21	1:C:409:HIS:CE1	2.43	0.54
1:C:603:ARG:NH1	1:C:603:ARG:HG3	2.20	0.53
1:F:584:LEU:CD2	1:F:588:LEU:HD12	2.38	0.53
1:E:424:VAL:HG12	1:E:424:VAL:O	2.09	0.53
1:H:388:LYS:HE3	1:H:392:GLU:CD	2.29	0.53
1:D:320:VAL:C	1:D:322:SER:H	2.13	0.53
1:F:325:PRO:HG2	4:F:892:HOH:O	2.08	0.53
1:G:300:SER:HB2	1:G:325:PRO:HG3	1.90	0.53
1:F:391:MET:HA	1:F:391:MET:CE	2.39	0.53
1:D:421:LEU:HD11	1:D:438:LEU:HD21	1.91	0.52
1:E:463:ASN:ND2	1:G:281:ARG:HH11	2.07	0.52
1:A:453:THR:HG23	4:A:963:HOH:O	2.08	0.52
1:D:549:GLU:OE2	1:D:556:VAL:HA	2.08	0.52
1:H:280:THR:HG22	1:H:281:ARG:N	2.24	0.52
1:B:463:ASN:HD22	1:D:281:ARG:NH1	2.07	0.52
1:D:363:ARG:HH11	1:D:363:ARG:CA	2.20	0.52
1:E:585:LEU:CD2	1:E:592:ILE:HD12	2.38	0.52
1:G:484:LEU:O	1:G:488:THR:HG23	2.10	0.52
1:E:600:ARG:O	1:E:604:GLU:HG3	2.10	0.52
1:B:280:THR:HB	1:B:282:ARG:NH1	2.24	0.51
1:E:309:ASP:HA	4:E:879:HOH:O	2.09	0.51
1:H:526:SER:HB2	1:H:599:LEU:HD22	1.90	0.51
1:H:539:LEU:HD11	1:H:566:VAL:HG13	1.92	0.51
1:G:304:ILE:HG21	1:G:315:PHE:CE1	2.41	0.51
1:G:376:VAL:HG22	1:G:521:ASP:HA	1.91	0.51
1:F:476:LEU:HB3	1:F:517:LEU:HD12	1.93	0.51
1:F:584:LEU:HD23	1:F:588:LEU:HD12	1.93	0.51
1:H:299:LYS:HD3	1:H:325:PRO:HB2	1.92	0.51
1:C:391:MET:HA	1:C:391:MET:HE2	1.91	0.51
1:B:388:LYS:H	1:B:388:LYS:CD	2.14	0.51
1:H:571:ILE:HB	1:H:572:PRO:HD3	1.92	0.51
1:H:594:GLU:N	1:H:595:PRO:HD2	2.26	0.50
1:A:303:ALA:HA	1:A:334:HIS:CE1	2.47	0.50
1:B:391:MET:HE3	1:B:394:LEU:HD12	1.94	0.50
1:B:447:PHE:CZ	1:B:470:LYS:HG3	2.47	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:603:ARG:NH1	1:E:603:ARG:HG3	2.25	0.50
1:E:351:TRP:O	1:E:355:VAL:HG23	2.11	0.50
1:E:571:ILE:CG2	1:E:603:ARG:HH12	2.20	0.50
1:H:327:VAL:O	1:H:331:VAL:HG23	2.11	0.50
1:A:468:GLU:OE2	1:A:506:LYS:HD2	2.11	0.50
1:E:468:GLU:OE2	1:E:506:LYS:HD2	2.11	0.50
1:E:482:MET:SD	1:E:518:HIS:HE1	2.35	0.50
1:G:306:THR:HG22	1:G:308:VAL:H	1.76	0.50
1:D:321:ALA:HA	1:D:327:VAL:CG2	2.41	0.50
1:F:324:VAL:HB	1:F:325:PRO:HD2	1.94	0.50
1:H:302:ALA:HB3	1:H:324:VAL:HG23	1.93	0.50
1:C:397:LEU:C	1:C:397:LEU:HD23	2.33	0.49
1:C:345:GLN:HA	1:C:345:GLN:NE2	2.26	0.49
1:D:369:ASN:OD1	1:D:371:ILE:HB	2.11	0.49
1:G:325:PRO:HG2	4:G:885:HOH:O	2.12	0.49
1:A:388:LYS:HB3	1:A:389:PRO:HD3	1.95	0.49
1:G:569:SER:HB2	4:G:922:HOH:O	2.10	0.49
1:D:316:ASP:O	1:D:320:VAL:HG23	2.12	0.49
1:E:567:GLU:HG2	1:E:609:LYS:CG	2.40	0.49
1:F:524:ALA:HB1	1:F:535:TRP:CD1	2.47	0.49
1:A:536:LEU:HD13	1:A:566:VAL:HG11	1.94	0.49
1:G:365:ASN:HB3	1:G:541:GLU:OE1	2.12	0.49
1:G:397:LEU:HD23	1:G:397:LEU:C	2.33	0.49
1:B:452:VAL:HB	1:B:455:PHE:CD2	2.48	0.49
1:D:329:GLN:HA	1:D:355:VAL:HG11	1.95	0.49
1:E:571:ILE:HB	1:E:572:PRO:HD3	1.95	0.49
1:G:603:ARG:HG3	1:G:603:ARG:HH11	1.76	0.49
1:G:603:ARG:NH2	4:G:847:HOH:O	2.46	0.49
1:B:324:VAL:HB	1:B:325:PRO:HD2	1.95	0.49
1:E:550:ARG:HG3	1:E:556:VAL:HG22	1.94	0.49
1:E:366:PRO:HD2	1:E:541:GLU:HG2	1.94	0.48
1:E:452:VAL:HB	1:E:455:PHE:CD2	2.48	0.48
1:F:304:ILE:HG13	1:F:310:LEU:HD21	1.95	0.48
1:H:397:LEU:C	1:H:397:LEU:HD23	2.33	0.48
1:A:516:LEU:HD23	1:A:585:LEU:HD21	1.94	0.48
1:B:344:SER:OG	1:B:347:GLU:HG3	2.13	0.48
1:E:289:GLN:NE2	1:E:292:ILE:HD11	2.28	0.48
1:F:299:LYS:HG3	4:F:876:HOH:O	2.12	0.48
1:C:310:LEU:HG	1:C:334:HIS:CD2	2.48	0.48
1:D:299:LYS:HD2	1:D:326:SER:OG	2.14	0.48
1:E:584:LEU:HA	1:E:587:GLN:NE2	2.28	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:296:VAL:HG23	1:E:356:ALA:HB1	1.94	0.48
1:F:485:HIS:HE1	1:F:581:THR:OG1	1.97	0.48
1:H:484:LEU:N	1:H:484:LEU:HD12	2.29	0.48
1:C:466:PHE:CE2	1:C:470:LYS:HD2	2.49	0.48
1:F:391:MET:HA	1:F:391:MET:HE3	1.94	0.48
1:F:458:THR:O	1:F:461:MET:HB2	2.13	0.48
1:A:571:ILE:HB	1:A:572:PRO:HD3	1.96	0.48
1:D:388:LYS:HB3	1:D:389:PRO:CD	2.44	0.48
1:G:411:VAL:O	1:G:412:CYS:HB2	2.14	0.48
1:G:452:VAL:HB	1:G:455:PHE:CD2	2.49	0.48
1:E:317:THR:CG2	1:E:375:ASP:OD1	2.62	0.47
1:G:282:ARG:HD3	1:G:282:ARG:C	2.34	0.47
1:B:568:LYS:HZ1	1:C:580:PRO:HB3	1.78	0.47
1:D:584:LEU:C	1:D:584:LEU:HD13	2.34	0.47
1:H:524:ALA:HB1	1:H:535:TRP:CD1	2.49	0.47
1:A:365:ASN:HB3	1:A:541:GLU:OE1	2.14	0.47
1:A:452:VAL:HB	1:A:455:PHE:CD2	2.49	0.47
1:A:568:LYS:CG	1:A:610:ALA:HB1	2.45	0.47
1:B:304:ILE:HG13	1:B:310:LEU:HD21	1.96	0.47
1:C:327:VAL:O	1:C:331:VAL:HG23	2.15	0.47
1:E:325:PRO:HG2	4:E:869:HOH:O	2.12	0.47
1:E:569:SER:O	1:E:572:PRO:HD2	2.15	0.47
1:E:584:LEU:HA	1:E:587:GLN:HE21	1.79	0.47
1:H:492:HIS:CB	1:H:584:LEU:HD21	2.45	0.47
1:H:569:SER:O	1:H:572:PRO:HD2	2.15	0.47
1:D:454:GLU:N	1:D:454:GLU:OE1	2.48	0.47
1:H:280:THR:HG22	1:H:281:ARG:H	1.79	0.47
1:C:577:PHE:O	1:C:580:PRO:HG2	2.15	0.46
1:G:603:ARG:NE	4:G:847:HOH:O	2.46	0.46
1:A:366:PRO:HD2	1:A:541:GLU:CG	2.46	0.46
1:B:351:TRP:O	1:B:355:VAL:HG23	2.15	0.46
1:D:320:VAL:O	1:D:324:VAL:HG12	2.14	0.46
1:C:372:HIS:O	1:C:376:VAL:HG23	2.16	0.46
1:G:363:ARG:HA	1:G:363:ARG:HD3	1.79	0.46
1:E:411:VAL:O	1:E:412:CYS:HB2	2.16	0.46
1:F:452:VAL:HB	1:F:455:PHE:CD2	2.49	0.46
1:B:325:PRO:HG2	4:B:911:HOH:O	2.16	0.46
1:F:475:HIS:CD2	1:F:514:SER:OG	2.69	0.46
1:B:354:LEU:HD21	1:B:404:PHE:HE2	1.81	0.46
1:D:318:PHE:O	1:D:321:ALA:HB3	2.16	0.46
1:E:324:VAL:HG22	1:E:325:PRO:CD	2.44	0.46



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:324:VAL:HG22	1:D:326:SER:H	1.81	0.46
1:B:327:VAL:O	1:B:331:VAL:HG23	2.17	0.45
1:H:441:LEU:HD23	1:H:441:LEU:O	2.15	0.45
1:C:345:GLN:HE21	1:C:345:GLN:CA	2.28	0.45
1:F:397:LEU:C	1:F:397:LEU:HD23	2.36	0.45
1:G:391:MET:HA	1:G:391:MET:HE2	1.98	0.45
1:A:324:VAL:HG22	4:A:903:HOH:O	2.15	0.45
1:C:492:HIS:CB	1:C:584:LEU:HD21	2.46	0.45
1:D:603:ARG:NH1	1:D:603:ARG:HG3	2.30	0.45
1:F:536:LEU:HD13	1:F:566:VAL:HG11	1.98	0.45
1:H:344:SER:OG	1:H:347:GLU:HG3	2.16	0.45
1:B:436:GLY:O	1:B:440:GLN:HG3	2.16	0.45
1:C:324:VAL:HB	1:C:325:PRO:HD2	1.99	0.45
1:D:376:VAL:HG22	1:D:521:ASP:HA	1.97	0.45
1:E:388:LYS:O	1:E:392:GLU:HG3	2.16	0.45
1:A:385:SER:HA	1:A:391:MET:HG3	1.99	0.45
1:C:576:PHE:O	1:C:576:PHE:CD2	2.69	0.45
1:B:366:PRO:HD2	1:B:541:GLU:HG2	1.97	0.45
1:A:354:LEU:HD21	1:A:404:PHE:CE2	2.52	0.45
1:A:539:LEU:HD11	1:A:566:VAL:HG13	1.99	0.45
1:D:309:ASP:OD1	1:D:312:ASP:HB3	2.16	0.45
1:F:475:HIS:O	1:F:479:HIS:HD2	2.00	0.45
1:B:397:LEU:HD23	1:B:397:LEU:C	2.37	0.45
1:D:328:LEU:HA	1:D:374:ALA:HB2	1.98	0.45
1:H:300:SER:O	1:H:301:CYS:HB2	2.17	0.45
1:C:603:ARG:NH1	1:C:603:ARG:CG	2.80	0.44
1:D:283:LEU:HB3	1:D:284:PRO:HD2	2.00	0.44
1:G:306:THR:HG22	1:G:307:ASP:N	2.32	0.44
1:A:447:PHE:CZ	1:A:470:LYS:HG3	2.51	0.44
1:A:597:HIS:O	1:A:601:LYS:HG3	2.18	0.44
1:C:321:ALA:N	1:C:327:VAL:HG21	2.32	0.44
1:F:568:LYS:HG2	1:F:610:ALA:HB1	2.00	0.44
1:H:585:LEU:HD23	1:H:585:LEU:O	2.17	0.44
1:A:568:LYS:HG2	1:A:610:ALA:HB1	1.99	0.44
1:C:325:PRO:HG2	4:C:861:HOH:O	2.16	0.44
1:D:584:LEU:HD13	1:D:584:LEU:O	2.17	0.44
1:H:595:PRO:O	1:H:599:LEU:HD22	2.17	0.44
1:H:354:LEU:HD21	1:H:404:PHE:CE2	2.53	0.44
1:A:358:VAL:HG11	1:A:407:LEU:CD2	2.48	0.44
1:B:336:ALA:HB1	1:B:342:PHE:CE2	2.52	0.44
1:D:351:TRP:O	1:D:355:VAL:HG23	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:376:VAL:HG21	1:D:409:HIS:CE1	2.52	0.44
1:F:582:PHE:CD2	1:F:595:PRO:HB2	2.53	0.44
1:G:324:VAL:HB	1:G:325:PRO:HD2	2.00	0.44
1:A:397:LEU:C	1:A:397:LEU:HD23	2.38	0.44
1:B:354:LEU:HD21	1:B:404:PHE:CE2	2.52	0.44
1:A:411:VAL:O	1:A:412:CYS:HB2	2.17	0.44
1:G:280:THR:HG22	1:G:280:THR:O	2.18	0.44
1:G:565:SER:OG	1:G:568:LYS:HB2	2.16	0.44
1:H:354:LEU:HD21	1:H:404:PHE:HE2	1.83	0.44
1:C:354:LEU:HB2	1:C:455:PHE:HB3	2.00	0.43
1:E:396:PRO:HG2	4:E:863:HOH:O	2.18	0.43
1:H:282:ARG:O	1:H:282:ARG:CG	2.65	0.43
1:D:411:VAL:O	1:D:412:CYS:HB2	2.18	0.43
1:G:594:GLU:N	1:G:595:PRO:HD2	2.34	0.43
1:B:411:VAL:O	1:B:412:CYS:HB2	2.18	0.43
1:C:388:LYS:N	1:C:389:PRO:HD2	2.33	0.43
1:F:281:ARG:HH21	1:H:463:ASN:ND2	2.10	0.43
1:A:593:GLU:HG2	1:A:597:HIS:CD2	2.53	0.43
1:C:475:HIS:O	1:C:479:HIS:HD2	2.00	0.43
1:D:452:VAL:HB	1:D:455:PHE:CD2	2.54	0.43
1:F:426:ASP:OD1	1:F:428:VAL:HG12	2.19	0.43
1:H:372:HIS:O	1:H:376:VAL:HG23	2.18	0.43
1:C:391:MET:HA	1:C:391:MET:HE3	2.00	0.43
1:D:332:ALA:HA	1:D:377:LEU:HD21	1.99	0.43
1:H:411:VAL:O	1:H:412:CYS:HB2	2.19	0.43
1:G:410:ASP:O	1:G:413:HIS:HB2	2.19	0.43
1:G:351:TRP:O	1:G:355:VAL:HG23	2.19	0.43
1:B:385:SER:HA	1:B:391:MET:HG3	2.00	0.43
1:C:579:ILE:N	1:C:580:PRO:HD2	2.34	0.43
1:G:571:ILE:HB	1:G:572:PRO:HD3	2.01	0.43
1:B:585:LEU:CD2	1:B:592:ILE:HD12	2.47	0.43
1:C:365:ASN:HB3	1:C:541:GLU:OE1	2.19	0.43
1:F:411:VAL:O	1:F:412:CYS:HB2	2.18	0.43
1:A:324:VAL:HG22	1:A:325:PRO:CD	2.48	0.42
1:A:447:PHE:CE1	1:A:470:LYS:HG3	2.54	0.42
1:E:426:ASP:OD1	$1:\overline{E:428:VAL:HG22}$	2.19	0.42
1:A:354:LEU:HD21	1:A:404:PHE:HE2	1.84	0.42
1:A:384:VAL:O	1:A:391:MET:HG2	2.18	0.42
1:D:481:ASP:CG	1:D:483:SER:HB3	2.39	0.42
1:F:376:VAL:HG22	1:F:521:ASP:HA	1.99	0.42
1:H:296:VAL:HG23	1:H:356:ALA:HB1	2.00	0.42



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:H:299:LYS:HD2	1:H:326:SER:HB2	2.01	0.42
1:C:595:PRO:HG2	4:C:834:HOH:O	2.19	0.42
1:D:288:VAL:HG11	1:D:441:LEU:HD11	2.02	0.42
1:F:447:PHE:CE1	1:F:470:LYS:HG3	2.53	0.42
1:G:345:GLN:HA	1:G:345:GLN:HE21	1.83	0.42
1:G:384:VAL:HG12	1:G:391:MET:CE	2.50	0.42
1:F:280:THR:HG22	1:F:280:THR:O	2.19	0.42
1:H:324:VAL:HG22	1:H:325:PRO:HD2	2.01	0.42
1:B:524:ALA:HB1	1:B:535:TRP:CD1	2.54	0.42
1:C:315:PHE:CD2	1:C:378:GLN:HG3	2.55	0.42
1:D:396:PRO:O	1:D:400:LYS:HG3	2.19	0.42
1:H:302:ALA:CB	1:H:324:VAL:HG23	2.50	0.42
1:B:570:GLN:O	1:B:573:PHE:HB3	2.20	0.42
1:D:466:PHE:CE2	1:D:470:LYS:HD2	2.55	0.42
1:D:594:GLU:N	1:D:595:PRO:HD2	2.34	0.42
1:F:396:PRO:HG2	4:F:965:HOH:O	2.19	0.42
1:E:384:VAL:HG12	1:E:391:MET:CE	2.50	0.42
1:F:610:ALA:HB3	1:F:612:VAL:HG23	2.02	0.42
1:B:579:ILE:HB	1:B:580:PRO:HD3	2.02	0.42
1:D:317:THR:HG22	1:D:371:ILE:HG23	2.01	0.42
1:D:545:GLN:O	1:D:549:GLU:HG3	2.20	0.42
1:F:571:ILE:HB	1:F:572:PRO:HD3	2.01	0.42
1:H:320:VAL:O	1:H:324:VAL:HG12	2.20	0.42
1:H:595:PRO:HG2	4:H:853:HOH:O	2.19	0.42
1:B:384:VAL:HG12	1:B:391:MET:HG2	2.02	0.41
1:D:527:ARG:HB3	1:D:531:ILE:HD12	2.02	0.41
1:E:579:ILE:HB	1:E:580:PRO:HD3	2.02	0.41
1:F:336:ALA:HB1	1:F:342:PHE:CE2	2.55	0.41
1:C:351:TRP:O	1:C:355:VAL:HG23	2.20	0.41
1:C:524:ALA:HB1	1:C:535:TRP:CD1	2.55	0.41
1:B:506:LYS:HE3	1:B:507:GLU:OE2	2.21	0.41
1:C:452:VAL:HB	1:C:455:PHE:CD2	2.55	0.41
1:D:346:GLU:HG2	1:D:350:LYS:HE3	2.03	0.41
1:D:354:LEU:O	1:D:358:VAL:HG23	2.21	0.41
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.91	0.41
1:B:310:LEU:HG	1:B:334:HIS:CD2	2.55	0.41
1:D:394:LEU:HD23	1:D:509:ARG:HD2	2.03	0.41
1:G:502:ASP:CG	1:G:504:THR:HG22	2.41	0.41
1:H:388:LYS:HB3	1:H:389:PRO:CD	2.50	0.41
1:B:585:LEU:O	1:B:585:LEU:HD23	2.21	0.41
1:F:435:LYS:HD3	4:F:947:HOH:O	2.19	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:344:SER:OG	1:D:347:GLU:HG3	2.21	0.41
1:F:579:ILE:HB	1:F:580:PRO:HD3	2.01	0.41
1:G:396:PRO:HG2	4:G:877:HOH:O	2.21	0.41
1:H:410:ASP:O	1:H:413:HIS:HB2	2.21	0.41
1:H:324:VAL:CG2	1:H:325:PRO:CD	2.98	0.41
1:A:323:ARG:HE	1:A:323:ARG:HB2	1.62	0.41
1:B:585:LEU:HD21	1:B:592:ILE:CD1	2.47	0.41
1:C:328:LEU:HA	1:C:374:ALA:HB2	2.03	0.41
1:C:583:ASP:O	1:C:587:GLN:HG2	2.21	0.41
1:D:576:PHE:CD2	1:D:576:PHE:O	2.74	0.41
1:F:390:LEU:HG	1:F:394:LEU:HD11	2.03	0.41
1:H:363:ARG:HA	1:H:363:ARG:HD3	1.95	0.41
1:C:350:LYS:HD3	1:C:456:ASP:O	2.21	0.41
1:A:492:HIS:HB2	1:A:584:LEU:HD21	2.03	0.40
1:D:388:LYS:HE3	1:D:392:GLU:CD	2.42	0.40
1:F:363:ARG:HB3	1:F:364:PRO:HD2	2.03	0.40
1:G:304:ILE:CG2	1:G:315:PHE:HE1	2.30	0.40
1:C:390:LEU:HD23	1:C:390:LEU:HA	1.92	0.40
1:H:397:LEU:HD23	1:H:397:LEU:O	2.21	0.40
1:C:586:HIS:HE1	1:C:593:GLU:HG2	1.79	0.40
1:D:315:PHE:CD2	1:D:378:GLN:HG3	2.57	0.40
1:E:310:LEU:CD1	1:E:334:HIS:HB3	2.51	0.40
1:E:462:ASP:OD2	1:E:464:ALA:HB3	2.21	0.40
1:F:512:ALA:O	1:F:516:LEU:HG	2.22	0.40
1:F:596:LEU:HD21	1:F:600:ARG:NH2	2.37	0.40
1:G:493:GLY:O	1:G:496:LEU:HB3	2.21	0.40
1:C:321:ALA:CA	1:C:327:VAL:CG2	2.99	0.40
1:D:295:VAL:HA	1:D:455:PHE:HZ	1.87	0.40
1:G:304:ILE:CD1	1:G:330:SER:HB3	2.51	0.40
1:H:462:ASP:HB3	1:H:465:SER:H	1.86	0.40
1:H:603:ARG:NH1	1:H:603:ARG:CG	2.84	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	325/345~(94%)	321 (99%)	3~(1%)	1 (0%)	41 37
1	В	331/345~(96%)	322~(97%)	9~(3%)	0	100 100
1	С	331/345~(96%)	324 (98%)	7 (2%)	0	100 100
1	D	320/345~(93%)	307 (96%)	11 (3%)	2 (1%)	25 19
1	Е	325/345~(94%)	314 (97%)	11 (3%)	0	100 100
1	F	332/345~(96%)	325~(98%)	6(2%)	1 (0%)	41 37
1	G	332/345~(96%)	328~(99%)	4 (1%)	0	100 100
1	Н	324/345~(94%)	311 (96%)	12 (4%)	1 (0%)	41 37
All	All	2620/2760~(95%)	2552 (97%)	63 (2%)	5(0%)	47 44

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

All (5) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	303	ALA
1	Н	302	ALA
1	D	485	HIS
1	F	301	CYS
1	D	321	ALA

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	273/286~(96%)	271~(99%)	2(1%)	84 88
1	В	276/286~(96%)	273~(99%)	3 (1%)	73 78
1	$\mathbf{C}$	276/286~(96%)	275 (100%)	1 (0%)	91 93
1	D	271/286~(95%)	269~(99%)	2(1%)	84 88
1	Ε	274/286~(96%)	270~(98%)	4 (2%)	65 69
1	F	277/286~(97%)	276 (100%)	1 (0%)	91 93



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	277/286~(97%)	276~(100%)	1 (0%)	91 93
1	Н	272/286~(95%)	266~(98%)	6 (2%)	52 55
All	All	2196/2288~(96%)	2176 (99%)	20 (1%)	78 83

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All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	310	LEU
1	А	391	MET
1	В	290	ASP
1	В	391	MET
1	В	533	ARG
1	С	533	ARG
1	D	363	ARG
1	D	533	ARG
1	Е	309	ASP
1	Е	317	THR
1	Е	318	PHE
1	Е	584	LEU
1	F	517	LEU
1	G	309	ASP
1	Н	282	ARG
1	Н	328	LEU
1	Н	462	ASP
1	Н	483	SER
1	Н	504	THR
1	Н	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	334	HIS
1	А	345	GLN
1	В	345	GLN
1	В	463	ASN
1	В	475	HIS
1	С	289	GLN
1	С	345	GLN
1	С	360	ASN
1	С	475	HIS



Mol	Chain	Res	Type
1	С	479	HIS
1	С	485	HIS
1	С	586	HIS
1	D	334	HIS
1	D	345	GLN
1	D	360	ASN
1	D	463	ASN
1	D	485	HIS
1	D	586	HIS
1	Е	289	GLN
1	Е	345	GLN
1	Е	360	ASN
1	Е	393	HIS
1	Е	463	ASN
1	Е	485	HIS
1	Е	587	GLN
1	F	289	GLN
1	F	345	GLN
1	F	475	HIS
1	F	479	HIS
1	F	485	HIS
1	F	597	HIS
1	G	345	GLN
1	G	463	ASN
1	Н	345	GLN
1	Н	463	ASN
1	Н	475	HIS
1	Н	485	HIS

#### 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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	329/345~(95%)	0.03	9 (2%) 54 53	3	12, 20, 38, 70	0
1	В	333/345~(96%)	0.16	13 (3%) 39 3	8	16, 25, 47, 72	0
1	С	333/345~(96%)	0.01	12 (3%) 42 4	2	13, 25, 50, 74	0
1	D	324/345~(93%)	0.78	43 (13%) 3	2	20,  45,  64,  69	0
1	Ε	329/345~(95%)	0.20	22 (6%) 17 1	7	17, 29, 61, 72	0
1	F	334/345~(96%)	0.06	11 (3%) 46 4	5	14, 22, 40, 68	0
1	G	334/345~(96%)	0.08	16 (4%) 30 2	9	15, 24, 46, 64	0
1	Н	328/345~(95%)	0.11	10 (3%) 50 4	9	17, 32, 54, 73	0
All	All	2644/2760~(95%)	0.18	136 (5%) 28 2	27	12, 27, 55, 74	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	612	VAL	8.9
1	В	610	ALA	8.7
1	С	612	VAL	7.9
1	Е	308	VAL	6.6
1	Е	302	ALA	6.6
1	А	280	THR	6.5
1	В	611	GLY	6.5
1	А	303	ALA	6.4
1	G	304	ILE	5.8
1	В	280	THR	5.7
1	Н	280	THR	5.6
1	F	613	THR	5.2
1	F	280	THR	5.1
1	G	280	THR	5.1
1	D	309	ASP	5.1
1	А	302	ALA	5.0



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1         D         556         VAL         4.8           1         E         282         ARG         4.6           1         D         280         THR         4.6           1         C         611         GLY         4.6           1         E         301         CYS         4.5           1         B         300         SER         4.4           1         E         576         PHE         4.3           1         C         576         PHE         4.3           1         D         308         VAL         4.3           1         D         303         ALA         4.1           1         D         303         ALA         4.1           1         D         343         ALA         4.1           1         D         560         PHE         4.0           1         D         560         PHE         4.0           1         D         550         ARG         4.0           1         D         576         PHE         4.0           1         D         576         PHE         4.0	IVI0I	Ullain	nes	туре	IIIII
1         E         282         ARG         4.6           1         D         280         THR         4.6           1         C         611         GLY         4.6           1         E         301         CYS         4.5           1         B         300         SER         4.4           1         E         576         PHE         4.3           1         C         576         PHE         4.3           1         D         308         VAL         4.3           1         D         300         SER         4.2           1         G         303         ALA         4.1           1         D         343         ALA         4.1           1         G         612         VAL         4.1           1         D         560         PHE         4.0           1         D         560         PHE         4.0           1         D         560         PHE         4.0           1         D         576         PHE         4.0           1         D         576         PHE         4.0	1	D	556	VAL	4.8
1       D       280       THR       4.6         1       C       611       GLY       4.6         1       E       301       CYS       4.5         1       B       300       SER       4.4         1       E       307       ASP       4.4         1       E       576       PHE       4.3         1       C       576       PHE       4.3         1       D       308       VAL       4.3         1       D       300       SER       4.2         1       G       303       ALA       4.1         1       D       343       ALA       4.1         1       G       612       VAL       4.1         1       B       609       LYS       4.1         1       D       560       PHE       4.0         1       D       560       PHE       4.0         1       D       560       PHE       4.0         1       D       576       PHE       4.0         1       D       304       ILE       3.0         1       D	1	Е	282	ARG	4.6
1       C $611$ GLY $4.6$ 1       E $301$ CYS $4.5$ 1       B $300$ SER $4.4$ 1       E $307$ ASP $4.4$ 1       E $576$ PHE $4.3$ 1       C $576$ PHE $4.3$ 1       D $308$ VAL $4.3$ 1       D $300$ SER $4.2$ 1       G $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       G $612$ VAL $4.1$ 1       D $560$ PHE $4.0$ 1       D $282$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3$	1	D	280	THR	4.6
1       E       301       CYS       4.5         1       B       300       SER       4.4         1       E       307       ASP       4.4         1       E       576       PHE       4.3         1       C       576       PHE       4.3         1       D       308       VAL       4.3         1       D       300       SER       4.2         1       G       303       ALA       4.1         1       D       343       ALA       4.1         1       G       612       VAL       4.1         1       B       609       LYS       4.1         1       D       560       PHE       4.0         1       D       560       PHE       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       D       576       PHE       4.0         1       D       576       PHE       4.0         1       D       310       LEU       3.9         1       E	1	С	611	GLY	4.6
1       B       300       SER       4.4         1       E       307       ASP       4.4         1       E       576       PHE       4.3         1       C       576       PHE       4.3         1       D       308       VAL       4.3         1       D       300       SER       4.2         1       G       303       ALA       4.1         1       D       343       ALA       4.1         1       G       612       VAL       4.1         1       B       609       LYS       4.1         1       D       560       PHE       4.0         1       D       560       PHE       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       D       576       PHE       4.0         1       D       310       LEU       3.9         1       E       565       SER       3.8         1       D       3	1	Е	301	CYS	4.5
1       E $307$ ASP $4.4$ 1       E $576$ PHE $4.3$ 1       D $308$ VAL $4.3$ 1       D $300$ SER $4.2$ 1       D $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $560$ PHE $4.0$ 1       D $560$ PHE $4.0$ 1       D $560$ PHE $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $576$ PHE $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       D $310$ LEU $3.9$ 1       B $349$ GLN $3$	1	В	300	SER	4.4
1       E $576$ PHE $4.3$ 1       D $308$ VAL $4.3$ 1       D $300$ SER $4.2$ 1       G $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $560$ PHE $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3.8$ 1       D $310$ LEU $3.9$ 1       E $300$ SER $3.7$ 1       G $300$ SER $3$	1	Е	307	ASP	4.4
1       C $576$ PHE $4.3$ 1       D $308$ VAL $4.3$ 1       D $300$ SER $4.2$ 1       G $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $560$ PHE $4.0$ 1       D $282$ ARG $4.0$ 1       D $282$ ARG $4.0$ 1       D $282$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $576$ PHE $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3.8$ 1       B $349$ GLN $3.8$ 1       G $300$ SER $3$	1	Е	576	PHE	4.3
1       D $308$ VAL $4.3$ 1       D $300$ SER $4.2$ 1       G $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       D $560$ PHE $4.0$ 1       D $560$ PHE $4.0$ 1       D $560$ PHE $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3.8$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3.8$ 1       C $280$ THR $3.7$ 1       G $300$ SER $3$	1	С	576	PHE	4.3
1       D       300       SER       4.2         1       G       303       ALA       4.1         1       D       343       ALA       4.1         1       D       343       ALA       4.1         1       D       612       VAL       4.1         1       D       560       PHE       4.0         1       D       282       ARG       4.0         1       D       282       ARG       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       D       576       PHE       4.0         1       D       310       LEU       3.9         1       E       565       SER       3.8         1       B       349       GLN       3.8         1       C       280       THR       3.7         1       G       300       SER       3.7         1       H       301       CYS       3.7         1       H       2	1	D	308	VAL	4.3
1       G $303$ ALA $4.1$ 1       D $343$ ALA $4.1$ 1       G $612$ VAL $4.1$ 1       D $560$ PHE $4.0$ 1       D $282$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       D $550$ ARG $4.0$ 1       A $304$ ILE $4.0$ 1       D $576$ PHE $4.0$ 1       D $310$ LEU $3.9$ 1       E $565$ SER $3.8$ 1       B $349$ GLN $3.8$ 1       C $280$ THR $3.7$ 1       H $301$ CYS $3.7$ 1       H $282$ ARG $3$	1	D	300	SER	4.2
1       D       343       ALA       4.1         1       G       612       VAL       4.1         1       B       609       LYS       4.1         1       D       560       PHE       4.0         1       D       282       ARG       4.0         1       D       282       ARG       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       A       302       ALA       4.0         1       A       304       ILE       4.0         1       D       576       PHE       4.0         1       D       310       LEU       3.9         1       E       565       SER       3.8         1       B       349       GLN       3.8         1       C       280       THR       3.7         1       G       300       SER       3.7         1       H       301       CYS       3.7         1       F       611       GLY       3.4         1       D       5	1	G	303	ALA	4.1
1       G       612       VAL       4.1         1       B       609       LYS       4.1         1       D       560       PHE       4.0         1       D       282       ARG       4.0         1       D       550       ARG       4.0         1       D       550       ARG       4.0         1       G       302       ALA       4.0         1       A       304       ILE       4.0         1       A       304       ILE       4.0         1       D       576       PHE       4.0         1       D       576       PHE       4.0         1       D       310       LEU       3.9         1       E       565       SER       3.8         1       B       349       GLN       3.8         1       C       280       THR       3.7         1       G       300       SER       3.7         1       H       301       CYS       3.7         1       F       611       GLY       3.4         1       D       5	1	D	343	ALA	4.1
1B $609$ LYS $4.1$ 1D $560$ PHE $4.0$ 1D $282$ ARG $4.0$ 1D $550$ ARG $4.0$ 1D $550$ ARG $4.0$ 1G $302$ ALA $4.0$ 1A $304$ ILE $4.0$ 1D $576$ PHE $4.0$ 1D $310$ LEU $3.9$ 1E $565$ SER $3.8$ 1C $280$ THR $3.7$ 1G $300$ SER $3.7$ 1H $301$ CYS $3.7$ 1H $301$ CYS $3.7$ 1H $282$ ARG $3.5$ 1F $611$ GLY $3.4$ 1D $566$ VAL $3.4$ 1D $561$ GLU $3.3$ 1H $308$ VAL $3.2$ 1D $567$ GLU $3.2$ 1D $567$ GLU $3.2$ 1H $303$ ALA $3.2$	1	G	612	VAL	4.1
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	609	LYS	4.1
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	560	PHE	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	282	ARG	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	550	ARG	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	302	ALA	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	304	ILE	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	576	PHE	4.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	310	LEU	3.9
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	565	SER	3.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	349	GLN	3.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	С	280	THR	3.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	300	SER	3.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Н	301	CYS	3.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Е	306	THR	3.5
1       F       611       GLY       3.4         1       D       566       VAL       3.4         1       D       323       ARG       3.4         1       D       323       ARG       3.4         1       A       611       GLY       3.4         1       D       561       GLU       3.3         1       H       308       VAL       3.2         1       D       346       GLU       3.2         1       D       567       GLU       3.2         1       H       303       ALA       3.2	1	Н	282	ARG	3.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	F	611	GLY	3.4
1         D         323         ARG         3.4           1         A         611         GLY         3.4           1         D         561         GLU         3.3           1         H         308         VAL         3.2           1         D         346         GLU         3.2           1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	D	566	VAL	3.4
1         A         611         GLY         3.4           1         D         561         GLU         3.3           1         H         308         VAL         3.2           1         D         346         GLU         3.2           1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	D	323	ARG	3.4
1         D         561         GLU         3.3           1         H         308         VAL         3.2           1         D         346         GLU         3.2           1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	А	611	GLY	3.4
1         H         308         VAL         3.2           1         D         346         GLU         3.2           1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	D	561	GLU	3.3
1         D         346         GLU         3.2           1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	Н	308	VAL	3.2
1         D         567         GLU         3.2           1         H         303         ALA         3.2	1	D	346	GLU	3.2
1 H 303 ALA 3.2	1	D	567	GLU	3.2
	1	Н	303	ALA	3.2
1   C   610   ALA   3.2	1	С	610	ALA	3.2
1 E 562 THR 3.2	1	Е	562	THR	3.2
1 C 608 ALA 3.1	1	С	608	ALA	3.1
1 D 606 TYR 3.1	1	D	606	TYR	3.1



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 Mol
 Chain
 Res
 Type
 RSRZ
 Image: Continued from previous page...

1	Е	563	PRO	3.1
1	Е	280	THR	3.1
1	G	306	THR	3.1
1	G	305	GLY	3.0
1	F	300	SER	3.0
1	Е	564	SER	3.0
1	G	613	THR	2.9
1	D	324	VAL	2.9
1	А	300	SER	2.9
1	Е	310	LEU	2.8
1	Н	345	GLN	2.8
1	D	564	SER	2.8
1	С	308	VAL	2.8
1	D	600	ARG	2.8
1	В	302	ALA	2.7
1	Н	302	ALA	2.7
1	D	344	SER	2.7
1	F	343	ALA	2.7
1	G	301	CYS	2.7
1	F	302	ALA	2.7
1	В	301	CYS	2.7
1	D	345	GLN	2.7
1	D	424	VAL	2.7
1	D	533	ARG	2.7
1	D	298	PRO	2.6
1	D	333	MET	2.6
1	D	342	PHE	2.6
1	В	343	ALA	2.6
1	С	571	ILE	2.5
1	G	343	ALA	2.5
1	Ε	300	SER	2.5
1	В	337	LEU	2.5
1	В	303	ALA	2.5
1	Е	566	VAL	2.5
1	C	304	ILE	2.5
1	F	$\overline{612}$	VAL	2.5
1	E	309	ASP	2.5
1	D	568	LYS	2.5
1	D	557	THR	2.4
1	D	497	SER	2.4
1	А	343	ALA	2.4
1	D	565	SER	2.3



Mol	Chain	Res	Type	RSRZ
1	D	563	PRO	2.3
1	F	609	LYS	2.3
1	А	282	ARG	2.3
1	С	307	ASP	2.3
1	F	345	GLN	2.3
1	D	528	GLY	2.3
1	G	307	ASP	2.3
1	D	605	LEU	2.2
1	Е	323	ARG	2.2
1	Н	343	ALA	2.2
1	С	573	PHE	2.2
1	А	345	GLN	2.2
1	D	328	LEU	2.2
1	D	554	LEU	2.2
1	G	337	LEU	2.2
1	Н	565	SER	2.2
1	D	551	ARG	2.2
1	G	482	MET	2.2
1	Н	333	MET	2.2
1	Е	606	TYR	2.2
1	Е	568	LYS	2.2
1	D	571	ILE	2.1
1	G	605	LEU	2.1
1	F	610	ALA	2.1
1	D	337	LEU	2.1
1	D	353	PHE	2.1
1	В	462	ASP	2.1
1	D	326	SER	2.1
1	F	282	ARG	2.1
1	С	306	THR	2.1
1	Е	610	ALA	2.0
1	Е	560	PHE	2.0
1	Е	597	HIS	2.0
1	G	342	PHE	2.0
1	D	602	LEU	2.0
1	D	425	GLN	2.0

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# 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 monosaccharides 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,  $95^{th}$  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
3	MG	D	702	1/1	0.94	0.15	31,31,31,31	0
3	MG	Е	702	1/1	0.94	0.10	26,26,26,26	0
3	MG	G	702	1/1	0.96	0.15	18,18,18,18	0
3	MG	В	702	1/1	0.97	0.16	21,21,21,21	0
3	MG	Н	702	1/1	0.97	0.18	$25,\!25,\!25,\!25$	0
3	MG	F	702	1/1	0.98	0.20	19,19,19,19	0
3	MG	А	702	1/1	0.98	0.20	18,18,18,18	0
2	ZN	D	701	1/1	0.98	0.08	34,34,34,34	0
2	ZN	В	701	1/1	0.99	0.07	21,21,21,21	0
2	ZN	Е	701	1/1	0.99	0.06	$25,\!25,\!25,\!25$	0
3	MG	С	702	1/1	0.99	0.16	$15,\!15,\!15,\!15$	0
2	ZN	G	701	1/1	0.99	0.09	22,22,22,22	0
2	ZN	С	701	1/1	1.00	0.08	19,19,19,19	0
2	ZN	F	701	1/1	1.00	0.10	20,20,20,20	0
2	ZN	A	701	1/1	1.00	0.10	18,18,18,18	0
2	ZN	Н	701	1/1	1.00	0.07	$25,\!25,\!25,\!25$	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

