



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 AM GMT

PDB ID : 2DZN  
Title : Crystal structure analysis of yeast Nas6p complexed with the proteasome subunit, rpt3  
Authors : Yokoyama, S.; Padmanabhan, B.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-09-29  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

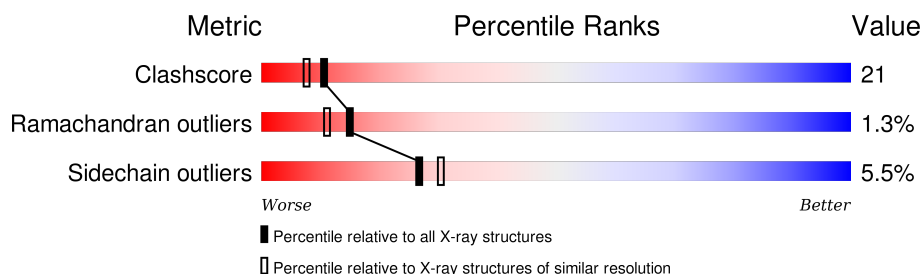
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	
1	C	228	
1	E	228	
2	B	82	
2	D	82	
2	F	82	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7346 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 Probable 26S proteasome regulatory subunit p28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1794	1151	305	332	6			
1	C	227	Total	C	N	O	S	0	0	0
			1800	1154	306	334	6			
1	E	227	Total	C	N	O	S	0	0	0
			1800	1154	306	334	6			

- Molecule 2 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	57	Total	C	N	O	S	0	0	0
			434	270	76	86	2			
2	D	67	Total	C	N	O	S	0	0	0
			515	321	92	100	2			
2	F	69	Total	C	N	O	S	0	0	0
			531	332	95	102	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	347	MET	-	INITIATING METHIONINE	UNP P33298
D	347	MET	-	INITIATING METHIONINE	UNP P33298
F	347	MET	-	INITIATING METHIONINE	UNP P33298

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	27	Total	O	0	0
			27	27		

*Continued on next page...*

*Continued from previous page...*

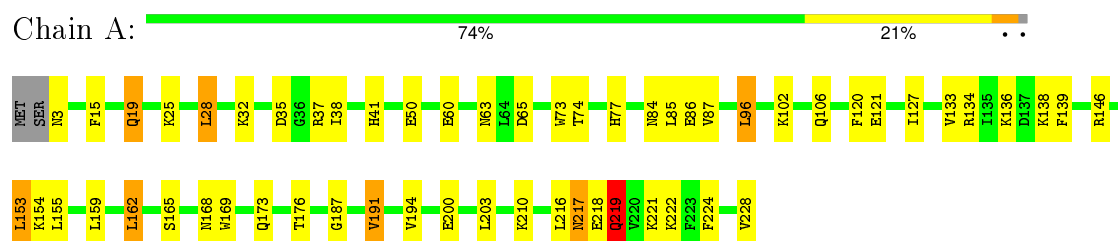
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	132	Total 132	O 132	0	0
3	D	35	Total 35	O 35	0	0
3	E	125	Total 125	O 125	0	0
3	F	11	Total 11	O 11	0	0

### 3 Residue-property plots [i](#)

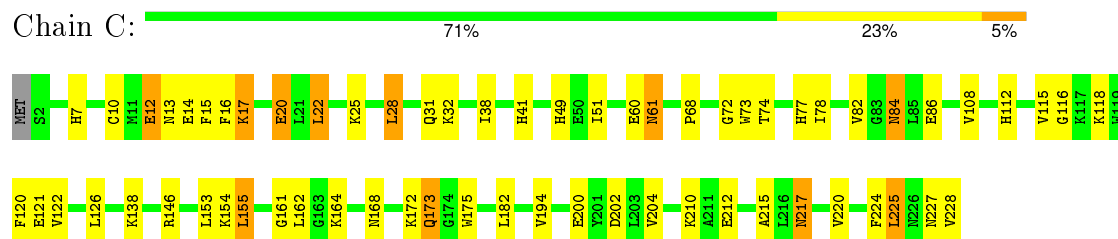
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

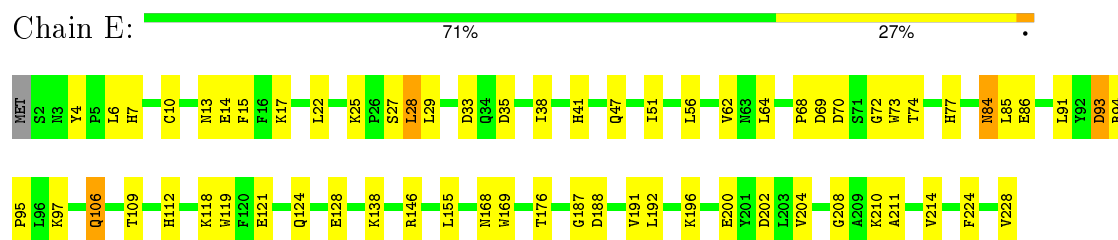
- Molecule 1: Probable 26S proteasome regulatory subunit p28



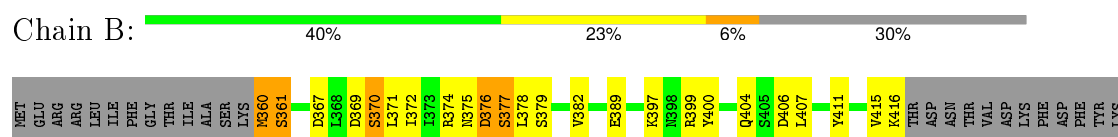
- Molecule 1: Probable 26S proteasome regulatory subunit p28



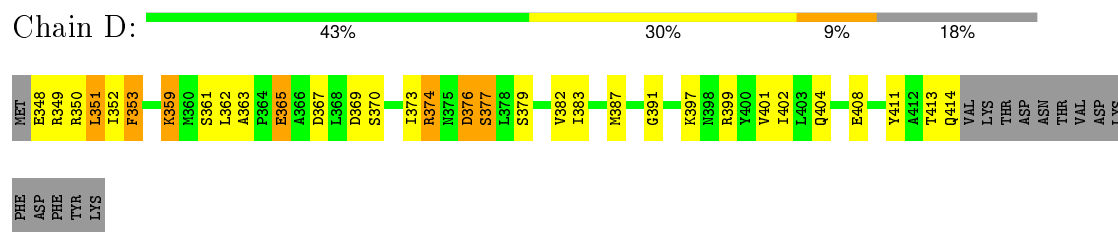
- Molecule 1: Probable 26S proteasome regulatory subunit p28



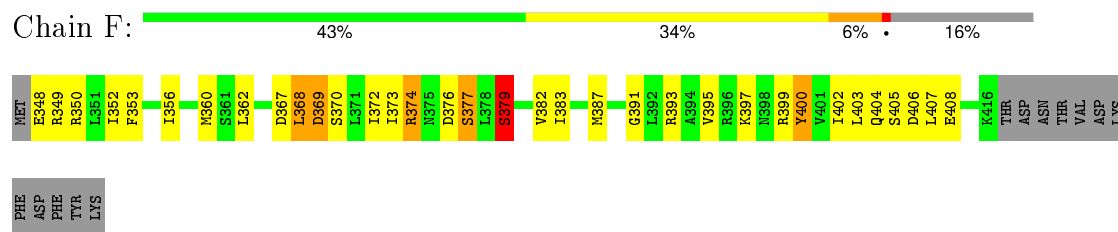
- Molecule 2: 26S protease regulatory subunit 6B homolog



- Molecule 2: 26S protease regulatory subunit 6B homolog



- Molecule 2: 26S protease regulatory subunit 6B homolog



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.38 Å   100.22 Å   72.20 Å 90.00°   94.70°   90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.1 (20.00-2.20)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.48	0/1837	0.69	3/2488 (0.1%)
1	C	0.46	0/1843	0.65	0/2496
1	E	0.43	0/1843	0.63	0/2496
2	B	0.41	0/436	0.68	0/588
2	D	0.43	0/518	0.75	1/697 (0.1%)
2	F	0.38	0/534	0.66	1/718 (0.1%)
All	All	0.44	0/7011	0.67	5/9483 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	N-CA-C	7.38	130.93	111.00
2	D	376	ASP	N-CA-C	7.12	130.22	111.00
1	A	134	ARG	N-CA-CB	-5.65	100.43	110.60
1	A	219	GLN	N-CA-C	-5.48	96.20	111.00
2	F	379	SER	N-CA-C	5.47	125.77	111.00

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	1794	0	1775	57	0
1	C	1800	0	1780	66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1800	0	1780	59	0
2	B	434	0	447	29	0
2	D	515	0	532	43	0
2	F	531	0	554	55	0
3	A	142	0	0	8	0
3	B	27	0	0	2	0
3	C	132	0	0	14	0
3	D	35	0	0	7	0
3	E	125	0	0	10	0
3	F	11	0	0	1	0
All	All	7346	0	6868	293	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 21.

All (293) 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)
2:F:349:ARG:NH2	2:F:377:SER:OG	1.66	1.26
2:F:349:ARG:NE	2:F:377:SER:HA	1.46	1.26
2:F:349:ARG:CZ	2:F:377:SER:HA	1.81	1.09
2:B:367:ASP:H	2:B:404:GLN:NE2	1.56	1.04
1:E:25:LYS:HE3	1:E:28:LEU:HD21	1.50	0.93
1:A:96:LEU:HD12	1:A:96:LEU:H	1.34	0.90
2:F:349:ARG:CZ	2:F:377:SER:CA	2.50	0.90
2:D:349:ARG:HG3	3:D:456:HOH:O	1.71	0.89
2:F:349:ARG:CZ	2:F:377:SER:OG	2.20	0.89
1:A:74:THR:H	1:A:77:HIS:HD2	1.14	0.87
2:F:349:ARG:HE	2:F:377:SER:HA	1.39	0.86
2:F:349:ARG:HD3	2:F:377:SER:H	1.39	0.86
2:F:349:ARG:NE	2:F:377:SER:CA	2.37	0.85
1:C:168:ASN:HD21	1:C:200:GLU:H	1.27	0.83
2:F:356:ILE:HG22	2:F:360:MET:HE1	1.62	0.82
2:D:367:ASP:H	2:D:404:GLN:NE2	1.77	0.82
1:A:73:TRP:CZ2	2:B:404:GLN:HG3	2.14	0.82
2:B:377:SER:HA	2:D:359:LYS:NZ	1.94	0.81
1:E:74:THR:H	1:E:77:HIS:HD2	1.26	0.81
1:E:64:LEU:HD21	1:E:94:ARG:HH12	1.48	0.79
2:F:369:ASP:O	2:F:373:ILE:HG22	1.83	0.78
1:E:25:LYS:HB2	1:E:28:LEU:CD2	2.14	0.78
1:C:146:ARG:NH1	3:C:356:HOH:O	2.17	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:349:ARG:CZ	2:D:349:ARG:HB2	2.14	0.75
2:B:367:ASP:H	2:B:404:GLN:HE21	1.29	0.75
2:B:376:ASP:O	2:B:377:SER:HB2	1.87	0.75
1:E:124:GLN:O	1:E:128:GLU:HG3	1.88	0.73
2:D:367:ASP:H	2:D:404:GLN:HE21	1.35	0.73
1:C:38:ILE:H	1:C:41:HIS:HD2	1.35	0.73
2:F:349:ARG:NH2	2:F:377:SER:CB	2.52	0.72
1:A:121:GLU:OE1	3:A:344:HOH:O	2.06	0.72
1:E:38:ILE:H	1:E:41:HIS:HD2	1.36	0.72
1:C:146:ARG:NE	3:C:357:HOH:O	2.23	0.72
1:A:38:ILE:H	1:A:41:HIS:HD2	1.35	0.71
2:D:349:ARG:NH1	2:D:349:ARG:HB2	2.06	0.71
1:E:25:LYS:O	1:E:28:LEU:HD22	1.90	0.71
1:A:84:ASN:HD22	1:A:87:VAL:H	1.37	0.71
1:A:133:VAL:HG22	1:A:159:LEU:HD22	1.74	0.70
1:C:182:LEU:HB3	3:C:343:HOH:O	1.91	0.70
2:F:367:ASP:OD2	2:F:370:SER:HB2	1.93	0.69
1:E:25:LYS:HB2	1:E:28:LEU:HD21	1.74	0.68
1:A:217:ASN:ND2	1:A:219:GLN:HB3	2.09	0.68
1:C:25:LYS:HE2	1:C:28:LEU:HD13	1.76	0.68
1:E:109:THR:H	1:E:112:HIS:CD2	2.12	0.68
1:C:74:THR:H	1:C:77:HIS:HD2	1.39	0.68
1:C:224:PHE:O	1:C:228:VAL:HG22	1.94	0.68
2:B:389:GLU:HG2	3:B:452:HOH:O	1.94	0.68
1:E:168:ASN:HD21	1:E:200:GLU:H	1.42	0.68
1:A:74:THR:H	1:A:77:HIS:CD2	2.06	0.67
1:E:106:GLN:O	1:E:138:LYS:HG2	1.95	0.66
2:D:348:GLU:HG2	2:D:348:GLU:O	1.96	0.66
2:B:367:ASP:N	2:B:404:GLN:NE2	2.39	0.65
1:E:138:LYS:HD3	3:E:322:HOH:O	1.97	0.65
1:C:168:ASN:ND2	1:C:200:GLU:H	1.93	0.65
1:A:60:GLU:HG2	3:A:296:HOH:O	1.95	0.65
1:A:63:ASN:ND2	1:A:65:ASP:HB2	2.11	0.65
2:D:413:THR:HB	2:D:414:GLN:OE1	1.96	0.65
2:B:371:LEU:HD11	2:B:407:LEU:HB3	1.79	0.65
2:D:374:ARG:HD2	2:D:411:TYR:CE2	2.32	0.65
2:F:349:ARG:CD	2:F:377:SER:H	2.10	0.64
2:F:404:GLN:O	2:F:408:GLU:HG2	1.97	0.64
1:E:121:GLU:CD	1:E:121:GLU:H	2.01	0.64
2:D:351:LEU:HD13	2:D:352:ILE:N	2.13	0.64
1:E:47:GLN:HG3	3:E:296:HOH:O	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:CD	1:C:121:GLU:H	2.00	0.63
2:D:359:LYS:HD3	2:D:359:LYS:O	1.98	0.63
1:A:217:ASN:HD21	1:A:219:GLN:HE21	1.46	0.63
2:D:348:GLU:OE1	2:D:373:ILE:HG22	1.97	0.63
2:D:353:PHE:CE1	2:D:383:ILE:HG12	2.33	0.63
1:C:217:ASN:ND2	1:C:220:VAL:H	1.95	0.63
1:E:188:ASP:HB2	3:E:235:HOH:O	1.98	0.63
2:B:416:LYS:HE2	2:B:416:LYS:HA	1.81	0.62
1:C:154:LYS:HG3	3:C:241:HOH:O	2.00	0.61
1:E:187:GLY:O	1:E:191:VAL:HG23	1.98	0.61
2:D:348:GLU:HB2	2:D:376:ASP:CG	2.21	0.61
1:A:187:GLY:O	1:A:191:VAL:HG13	2.00	0.61
1:C:16:PHE:O	1:C:17:LYS:CB	2.48	0.61
2:F:370:SER:O	2:F:374:ARG:HB2	2.01	0.60
1:E:168:ASN:ND2	1:E:200:GLU:H	1.99	0.60
1:E:74:THR:H	1:E:77:HIS:CD2	2.15	0.60
1:E:64:LEU:CD2	1:E:94:ARG:HH12	2.15	0.59
1:A:139:PHE:CZ	2:B:374:ARG:HD3	2.38	0.59
2:F:349:ARG:NH2	2:F:377:SER:HA	2.18	0.58
1:E:25:LYS:HB2	1:E:28:LEU:HD22	1.86	0.58
2:B:399:ARG:NH2	2:B:406:ASP:OD2	2.34	0.58
2:F:399:ARG:NH2	2:F:406:ASP:OD2	2.37	0.58
1:C:61:ASN:H	1:C:61:ASN:HD22	1.52	0.58
1:E:4:TYR:CE2	1:E:33:ASP:HA	2.39	0.58
1:C:161:GLY:HA3	3:C:360:HOH:O	2.03	0.57
1:C:217:ASN:C	1:C:217:ASN:HD22	2.07	0.57
1:A:173:GLN:NE2	2:B:374:ARG:O	2.38	0.57
1:A:224:PHE:CE1	1:A:228:VAL:HG11	2.39	0.57
2:F:349:ARG:CZ	2:F:377:SER:CB	2.82	0.57
2:D:351:LEU:C	2:D:351:LEU:HD13	2.25	0.57
2:F:400:TYR:H	2:F:400:TYR:HD2	1.53	0.57
2:B:411:TYR:CE1	2:B:415:VAL:HG21	2.40	0.57
1:A:96:LEU:CD1	1:A:96:LEU:H	2.13	0.57
1:A:96:LEU:N	1:A:96:LEU:HD12	2.14	0.57
1:E:192:LEU:HD11	1:E:196:LYS:HD3	1.87	0.56
2:F:349:ARG:HA	2:F:352:ILE:HD12	1.86	0.56
1:A:146:ARG:HD2	3:A:295:HOH:O	2.04	0.56
1:C:73:TRP:CZ2	2:D:404:GLN:HG3	2.40	0.56
2:F:362:LEU:HD12	2:F:402:ILE:HB	1.87	0.56
2:B:367:ASP:OD2	2:B:370:SER:HB2	2.06	0.56
1:E:95:PRO:HD2	3:E:246:HOH:O	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:HD21	1:A:65:ASP:HB2	1.71	0.56
1:C:84:ASN:C	1:C:84:ASN:HD22	2.10	0.56
1:E:109:THR:H	1:E:112:HIS:HD2	1.53	0.55
1:E:86:GLU:HA	1:E:86:GLU:OE2	2.06	0.55
1:E:119:TRP:HB3	3:E:327:HOH:O	2.05	0.55
2:F:360:MET:CE	2:F:387:MET:HB3	2.38	0.55
2:D:367:ASP:N	2:D:404:GLN:NE2	2.51	0.55
2:F:348:GLU:OE1	2:F:352:ILE:HD11	2.08	0.54
2:F:349:ARG:NH2	2:F:377:SER:CA	2.70	0.54
2:F:391:GLY:HA2	2:F:402:ILE:HD11	1.89	0.54
1:A:32:LYS:HE3	3:A:292:HOH:O	2.07	0.54
2:D:359:LYS:HD3	2:D:359:LYS:C	2.28	0.54
1:E:38:ILE:H	1:E:41:HIS:CD2	2.21	0.54
2:D:387:MET:HE3	3:D:442:HOH:O	2.07	0.54
1:A:106:GLN:O	1:A:138:LYS:HG2	2.08	0.54
2:D:348:GLU:HB2	2:D:376:ASP:HB3	1.89	0.54
1:A:73:TRP:HZ2	2:B:404:GLN:HG3	1.70	0.54
1:E:118:LYS:HA	1:E:155:LEU:HD11	1.90	0.54
2:F:348:GLU:HG2	2:F:349:ARG:N	2.23	0.53
2:B:360:MET:HB2	2:B:400:TYR:O	2.08	0.53
2:F:379:SER:OG	2:F:382:VAL:HG23	2.08	0.53
1:A:38:ILE:H	1:A:41:HIS:CD2	2.21	0.53
1:E:106:GLN:C	1:E:138:LYS:HG2	2.29	0.53
1:E:93:ASP:CG	1:E:93:ASP:O	2.46	0.53
1:A:218:GLU:HA	1:A:221:LYS:HB3	1.91	0.53
1:C:212:GLU:HG2	3:C:247:HOH:O	2.08	0.53
1:A:65:ASP:O	1:A:102:LYS:HE2	2.08	0.53
2:F:360:MET:SD	2:F:387:MET:HB3	2.49	0.53
1:C:61:ASN:ND2	1:C:61:ASN:H	2.06	0.53
1:E:68:PRO:HB2	1:E:72:GLY:HA2	1.91	0.52
1:A:133:VAL:HG11	1:A:165:SER:HB2	1.91	0.52
1:E:56:LEU:HD11	1:E:91:LEU:HD23	1.90	0.52
2:B:369:ASP:HA	2:B:372:ILE:HG12	1.90	0.52
1:C:61:ASN:N	1:C:61:ASN:HD22	2.07	0.52
1:C:116:GLY:HA3	3:C:310:HOH:O	2.09	0.52
1:A:41:HIS:HE1	1:A:73:TRP:O	1.92	0.52
2:F:356:ILE:O	2:F:360:MET:HE2	2.10	0.52
2:B:377:SER:HA	2:D:359:LYS:HZ1	1.71	0.51
1:A:168:ASN:HD21	1:A:200:GLU:H	1.58	0.51
2:B:375:ASN:HD21	2:B:378:LEU:HD21	1.75	0.51
1:A:15:PHE:CD1	1:A:50:GLU:HG2	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HE1	1:A:102:LYS:O	1.93	0.51
1:E:121:GLU:OE2	3:E:328:HOH:O	2.19	0.51
2:F:393:ARG:HD3	2:F:406:ASP:HA	1.92	0.51
1:A:153:LEU:HD21	3:A:369:HOH:O	2.09	0.51
2:F:395:VAL:C	2:F:397:LYS:H	2.13	0.51
1:A:136:LYS:HE2	1:A:169:TRP:CE3	2.46	0.51
1:C:215:ALA:HB2	3:C:343:HOH:O	2.10	0.51
2:D:348:GLU:HB2	2:D:376:ASP:OD1	2.11	0.51
1:C:146:ARG:CZ	3:C:357:HOH:O	2.58	0.51
2:F:399:ARG:NH1	2:F:403:LEU:HD12	2.27	0.50
2:D:349:ARG:HD3	3:D:429:HOH:O	2.11	0.50
1:E:22:LEU:HD21	1:E:29:LEU:HD13	1.92	0.50
1:C:15:PHE:HA	1:C:51:ILE:CD1	2.41	0.50
1:A:210:LYS:HE2	3:A:356:HOH:O	2.11	0.50
1:C:122:VAL:O	1:C:126:LEU:HG	2.12	0.50
1:E:97:LYS:HE3	3:E:253:HOH:O	2.11	0.50
2:D:348:GLU:HB2	2:D:376:ASP:CB	2.41	0.50
1:C:84:ASN:HD21	1:C:86:GLU:HB2	1.77	0.50
1:E:7:HIS:CD2	1:E:33:ASP:HB3	2.46	0.50
2:D:397:LYS:HD2	2:D:399:ARG:NH2	2.26	0.50
1:C:228:VAL:HG23	1:C:228:VAL:OXT	2.10	0.49
1:E:109:THR:OG1	1:E:112:HIS:HD2	1.94	0.49
2:D:350:ARG:NH2	2:D:369:ASP:OD1	2.45	0.49
1:E:64:LEU:HD21	1:E:94:ARG:NH1	2.22	0.49
1:E:85:LEU:HD22	1:E:121:GLU:HB3	1.94	0.49
2:D:376:ASP:O	2:D:377:SER:HB2	2.12	0.49
1:A:133:VAL:HG13	1:A:133:VAL:O	2.12	0.49
1:C:12:GLU:O	1:C:14:GLU:HG3	2.12	0.49
1:C:60:GLU:HG2	3:C:238:HOH:O	2.12	0.49
2:F:362:LEU:HD11	2:F:407:LEU:HD11	1.93	0.49
1:E:211:ALA:O	1:E:214:VAL:HG22	2.12	0.49
2:F:348:GLU:C	2:F:350:ARG:H	2.16	0.49
1:C:20:GLU:C	1:C:20:GLU:OE1	2.51	0.48
2:B:367:ASP:O	2:B:370:SER:HB3	2.14	0.48
1:C:115:VAL:HG13	1:C:155:LEU:HG	1.95	0.48
1:A:168:ASN:ND2	1:A:200:GLU:H	2.11	0.48
2:F:356:ILE:HG22	2:F:360:MET:CE	2.39	0.48
1:C:204:VAL:HG12	1:C:210:LYS:HG3	1.96	0.48
2:B:361:SER:HA	3:D:429:HOH:O	2.14	0.48
2:F:353:PHE:CD2	2:F:368:LEU:HD11	2.49	0.48
1:A:60:GLU:O	1:A:96:LEU:HD11	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ASN:HD21	1:C:200:GLU:N	2.05	0.48
1:C:25:LYS:HG3	1:C:28:LEU:HD22	1.96	0.48
2:D:363:ALA:HB2	2:D:401:VAL:CG1	2.43	0.48
1:C:146:ARG:NH2	3:C:357:HOH:O	2.46	0.47
1:C:120:PHE:HD1	1:C:155:LEU:HD13	1.79	0.47
1:E:73:TRP:CZ2	2:F:404:GLN:HG3	2.49	0.47
1:A:32:LYS:HA	1:A:37:ARG:O	2.13	0.47
2:F:379:SER:O	2:F:383:ILE:HG13	2.13	0.47
1:C:118:LYS:HB2	3:C:313:HOH:O	2.14	0.47
1:E:169:TRP:O	1:E:176:THR:HA	2.15	0.47
1:C:16:PHE:O	1:C:17:LYS:HB3	2.14	0.47
2:F:349:ARG:HH22	2:F:377:SER:HG	1.58	0.47
1:A:194:VAL:HG11	1:A:228:VAL:HB	1.96	0.47
2:D:348:GLU:N	2:D:377:SER:HG	2.13	0.46
1:A:139:PHE:CE1	2:B:374:ARG:HD3	2.50	0.46
1:A:219:GLN:HB3	1:A:219:GLN:HE21	1.62	0.46
1:C:84:ASN:HD22	1:C:86:GLU:H	1.62	0.46
1:C:162:LEU:HD22	1:C:162:LEU:N	2.31	0.46
2:F:348:GLU:O	2:F:350:ARG:N	2.44	0.46
1:E:204:VAL:CG1	1:E:208:GLY:HA2	2.46	0.46
2:D:379:SER:OG	2:D:382:VAL:HG23	2.16	0.46
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.71	0.46
1:A:84:ASN:HD21	1:A:86:GLU:HB3	1.81	0.45
1:A:84:ASN:ND2	1:A:87:VAL:H	2.10	0.45
1:A:35:ASP:OD2	2:B:399:ARG:HD3	2.16	0.45
1:E:93:ASP:HB3	3:E:348:HOH:O	2.16	0.45
1:E:146:ARG:NH2	2:F:367:ASP:OD1	2.49	0.45
2:F:362:LEU:CD1	2:F:402:ILE:HB	2.47	0.45
1:A:106:GLN:NE2	3:A:370:HOH:O	2.48	0.45
1:A:176:THR:HG21	1:A:203:LEU:HD12	1.99	0.45
1:C:68:PRO:HB2	1:C:72:GLY:HA2	1.99	0.45
1:A:85:LEU:HD22	1:A:121:GLU:HB3	1.99	0.45
1:E:35:ASP:OD1	2:F:399:ARG:NH1	2.49	0.45
1:C:224:PHE:CZ	1:C:228:VAL:HG21	2.52	0.45
1:A:216:LEU:HG	2:D:361:SER:HB3	1.99	0.45
2:B:397:LYS:NZ	3:B:443:HOH:O	2.47	0.44
1:C:12:GLU:H	1:C:12:GLU:HG2	1.58	0.44
2:F:399:ARG:NH2	2:F:406:ASP:OD1	2.50	0.44
2:D:365:GLU:H	2:D:365:GLU:HG3	1.45	0.44
3:E:315:HOH:O	2:F:397:LYS:HD2	2.17	0.44
2:F:391:GLY:HA2	2:F:402:ILE:CD1	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:LEU:HD12	2:D:352:ILE:HG13	2.00	0.44
1:C:78:ILE:O	1:C:82:VAL:HG23	2.17	0.44
1:E:202:ASP:HA	1:E:210:LYS:HD2	2.00	0.44
2:F:367:ASP:H	2:F:404:GLN:HE21	1.66	0.44
1:C:112:HIS:HD2	1:C:146:ARG:HH11	1.65	0.44
2:B:404:GLN:NE2	2:B:407:LEU:HD12	2.33	0.43
1:E:25:LYS:NZ	3:E:311:HOH:O	2.51	0.43
1:E:6:LEU:HD23	1:E:28:LEU:HB3	1.99	0.43
2:D:387:MET:CE	3:D:442:HOH:O	2.66	0.43
1:C:31:GLN:HG2	1:C:32:LYS:N	2.33	0.43
2:D:369:ASP:O	2:D:370:SER:C	2.57	0.43
1:C:200:GLU:HB3	1:C:202:ASP:OD1	2.19	0.43
1:E:14:GLU:OE2	1:E:17:LYS:HD3	2.18	0.43
1:A:133:VAL:HG22	1:A:159:LEU:CD2	2.44	0.43
1:E:7:HIS:O	1:E:10:CYS:N	2.50	0.43
1:A:218:GLU:CD	1:A:221:LYS:HD3	2.39	0.43
1:E:62:VAL:O	1:E:94:ARG:NH2	2.51	0.43
1:A:15:PHE:CE1	1:A:50:GLU:HG2	2.53	0.43
1:C:112:HIS:HD2	1:C:146:ARG:NH1	2.16	0.43
2:D:391:GLY:HA2	2:D:402:ILE:HD11	2.00	0.43
1:C:173:GLN:HG2	3:D:432:HOH:O	2.19	0.42
2:F:350:ARG:HG3	3:F:179:HOH:O	2.19	0.42
1:E:15:PHE:HD1	1:E:51:ILE:HG12	1.84	0.42
1:C:84:ASN:HB3	3:C:307:HOH:O	2.18	0.42
1:E:118:LYS:HA	1:E:155:LEU:CD1	2.50	0.42
1:E:25:LYS:O	1:E:28:LEU:CD2	2.65	0.42
1:C:112:HIS:CD2	1:C:146:ARG:NH1	2.88	0.42
1:C:74:THR:H	1:C:77:HIS:CD2	2.27	0.42
2:D:348:GLU:N	2:D:376:ASP:HB3	2.35	0.42
1:C:84:ASN:HD22	1:C:86:GLU:N	2.17	0.42
1:A:153:LEU:HD22	3:A:245:HOH:O	2.19	0.42
1:A:19:GLN:HB2	1:A:19:GLN:HE21	1.48	0.42
1:C:22:LEU:HA	1:C:22:LEU:HD13	1.84	0.42
1:A:25:LYS:O	1:A:28:LEU:HB2	2.20	0.42
2:B:377:SER:HA	2:D:359:LYS:HZ2	1.81	0.42
1:E:35:ASP:O	1:E:69:ASP:HB2	2.20	0.42
1:C:78:ILE:HG23	2:D:365:GLU:HG2	2.01	0.42
1:E:84:ASN:HD22	1:E:84:ASN:C	2.24	0.42
1:E:224:PHE:CE1	1:E:228:VAL:HG11	2.55	0.42
1:C:61:ASN:ND2	1:C:61:ASN:N	2.66	0.41
2:D:362:LEU:O	2:D:363:ALA:C	2.57	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:LYS:C	1:E:27:SER:H	2.23	0.41
2:F:348:GLU:CG	2:F:349:ARG:N	2.81	0.41
1:C:84:ASN:ND2	1:C:86:GLU:HB2	2.35	0.41
2:F:360:MET:HE1	2:F:387:MET:HB3	2.02	0.41
1:C:175:TRP:CZ3	2:D:376:ASP:OD1	2.74	0.41
1:C:172:LYS:HA	1:C:172:LYS:HD2	1.93	0.41
1:A:120:PHE:CD1	1:A:154:LYS:HG2	2.56	0.41
2:F:349:ARG:NE	2:F:377:SER:N	2.69	0.41
1:A:133:VAL:O	1:A:133:VAL:CG1	2.68	0.41
2:D:408:GLU:HG3	3:D:434:HOH:O	2.20	0.41
2:F:348:GLU:O	2:F:349:ARG:HB2	2.21	0.41
1:A:127:ILE:CG2	1:A:162:LEU:HD13	2.50	0.41
2:F:368:LEU:HD12	2:F:372:ILE:HD11	2.03	0.40
2:F:348:GLU:CG	2:F:349:ARG:H	2.33	0.40
2:F:405:SER:HA	2:F:408:GLU:CG	2.51	0.40
2:D:348:GLU:OE1	2:D:373:ILE:CG2	2.67	0.40
1:C:217:ASN:C	1:C:217:ASN:ND2	2.74	0.40
2:B:397:LYS:HD3	2:B:397:LYS:HA	1.93	0.40
1:C:227:ASN:N	3:C:351:HOH:O	2.54	0.40
2:B:375:ASN:O	2:B:376:ASP:C	2.59	0.40
1:C:16:PHE:O	1:C:17:LYS:HB2	2.22	0.40
2:B:379:SER:OG	2:B:382:VAL:HG23	2.22	0.40
1:C:7:HIS:O	1:C:10:CYS:HB2	2.21	0.40
1:C:194:VAL:HG11	1:C:228:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	224/228 (98%)	217 (97%)	7 (3%)	0	<b>100</b> <b>100</b>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	225/228 (99%)	214 (95%)	8 (4%)	3 (1%)	15	11
1	E	225/228 (99%)	211 (94%)	13 (6%)	1 (0%)	39	42
2	B	55/82 (67%)	46 (84%)	7 (13%)	2 (4%)	4	2
2	D	65/82 (79%)	58 (89%)	4 (6%)	3 (5%)	3	1
2	F	67/82 (82%)	58 (87%)	7 (10%)	2 (3%)	5	2
All	All	861/930 (93%)	804 (93%)	46 (5%)	11 (1%)	15	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	377	SER
2	F	374	ARG
2	F	379	SER
2	B	376	ASP
1	C	17	LYS
2	D	351	LEU
1	C	13	ASN
1	C	49	HIS
2	D	374	ARG
2	D	377	SER
1	E	70	ASP

### 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	196/198 (99%)	185 (94%)	11 (6%)	26	29
1	C	197/198 (100%)	183 (93%)	14 (7%)	18	19
1	E	197/198 (100%)	192 (98%)	5 (2%)	55	67
2	B	46/69 (67%)	43 (94%)	3 (6%)	21	23
2	D	54/69 (78%)	51 (94%)	3 (6%)	26	29
2	F	56/69 (81%)	51 (91%)	5 (9%)	12	11

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	746/801 (93%)	705 (94%)	41 (6%)	27	30

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	19	GLN
1	A	28	LEU
1	A	96	LEU
1	A	153	LEU
1	A	155	LEU
1	A	162	LEU
1	A	191	VAL
1	A	217	ASN
1	A	219	GLN
1	A	222	LYS
2	B	360	MET
2	B	361	SER
2	B	370	SER
1	C	12	GLU
1	C	20	GLU
1	C	22	LEU
1	C	28	LEU
1	C	61	ASN
1	C	84	ASN
1	C	108	VAL
1	C	138	LYS
1	C	153	LEU
1	C	155	LEU
1	C	164	LYS
1	C	173	GLN
1	C	217	ASN
1	C	225	LEU
2	D	353	PHE
2	D	359	LYS
2	D	365	GLU
1	E	13	ASN
1	E	28	LEU
1	E	84	ASN
1	E	93	ASP
1	E	106	GLN
2	F	368	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	369	ASP
2	F	376	ASP
2	F	377	SER
2	F	400	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	19	GLN
1	A	41	HIS
1	A	63	ASN
1	A	77	HIS
1	A	84	ASN
1	A	168	ASN
1	A	173	GLN
1	A	186	HIS
1	A	206	ASN
1	A	217	ASN
1	A	219	GLN
1	A	226	ASN
2	B	404	GLN
2	B	414	GLN
1	C	8	GLN
1	C	19	GLN
1	C	41	HIS
1	C	47	GLN
1	C	61	ASN
1	C	77	HIS
1	C	84	ASN
1	C	140	ASN
1	C	168	ASN
1	C	173	GLN
1	C	206	ASN
1	C	217	ASN
1	C	226	ASN
2	D	388	GLN
2	D	404	GLN
1	E	3	ASN
1	E	13	ASN
1	E	19	GLN
1	E	23	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	41	HIS
1	E	77	HIS
1	E	84	ASN
1	E	106	GLN
1	E	112	HIS
1	E	168	ASN
1	E	186	HIS
1	E	206	ASN
1	E	226	ASN
2	F	404	GLN
2	F	414	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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