



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:49 am BST

PDB ID : 1FCC  
Title : CRYSTAL STRUCTURE OF THE C2 FRAGMENT OF STREPTOCOCCAL PROTEIN G IN COMPLEX WITH THE FC DOMAIN OF HUMAN IGG  
Authors : Sauer-Eriksson, A.E.; Kleywegt, G.J.; Uhlen, M.; Jones, T.A.  
Deposited on : 1995-01-17  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

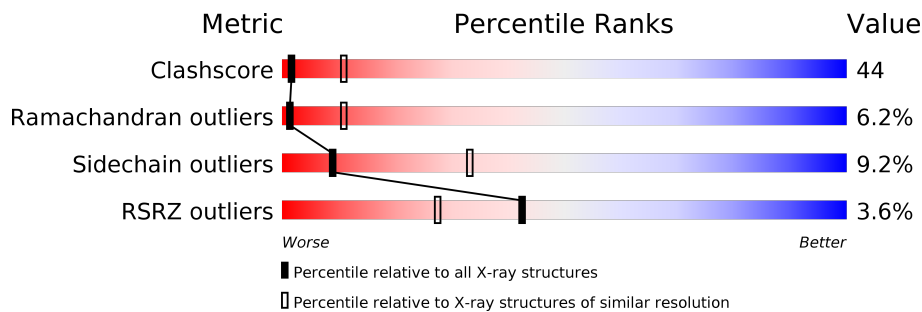
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	206	 9% 36% 53% 10%
1	B	206	 9% 38% 52% 9%
2	C	56	 34% 59% 7%
2	D	56	 36% 57% 7%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4180 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 IGG1 MO61 FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	Total 1656	C 1054	N 281	O 314	S 7	0	0	0
1	B	206	Total 1656	C 1054	N 281	O 314	S 7	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	CONFLICT	UNP P01857
A	283	GLN	GLU	CONFLICT	UNP P01857
A	294	GLN	GLU	CONFLICT	UNP P01857
A	312	ASN	ASP	CONFLICT	UNP P01857
A	315	ASP	ASN	CONFLICT	UNP P01857
A	356	GLU	ASP	CONFLICT	UNP P01857
A	358	MET	LEU	CONFLICT	UNP P01857
B	272	GLN	GLU	CONFLICT	UNP P01857
B	283	GLN	GLU	CONFLICT	UNP P01857
B	294	GLN	GLU	CONFLICT	UNP P01857
B	312	ASN	ASP	CONFLICT	UNP P01857
B	315	ASP	ASN	CONFLICT	UNP P01857
B	356	GLU	ASP	CONFLICT	UNP P01857
B	358	MET	LEU	CONFLICT	UNP P01857

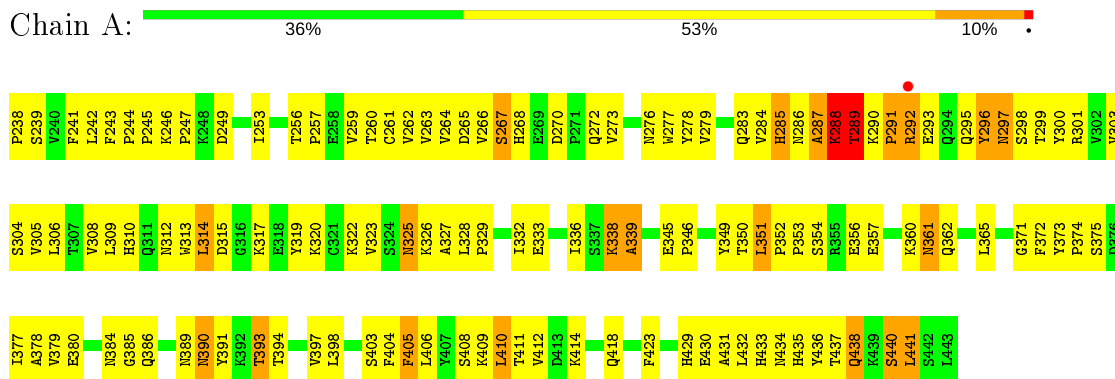
- Molecule 2 is a protein called STREPTOCOCCAL PROTEIN G (C2 FRAGMENT).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	56	Total 434	C 271	N 67	O 96	0	0	0
2	D	56	Total 434	C 271	N 67	O 96	0	0	0

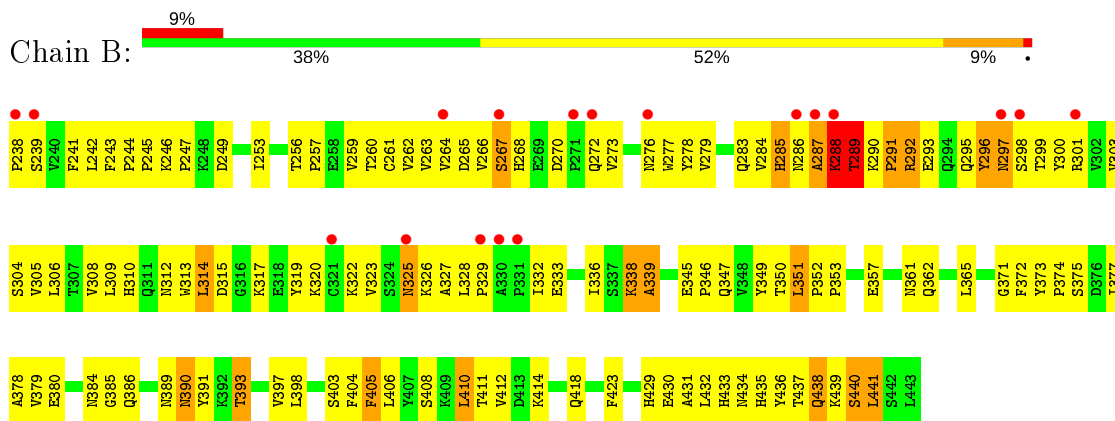
### 3 Residue-property plots

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.

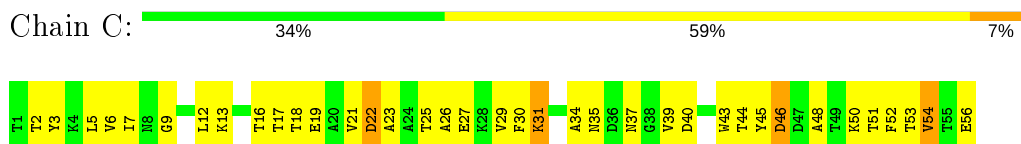
- Molecule 1: IGG1 MO61 FC



- Molecule 1: IGG1 MO61 FC



- Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)



- Molecule 2: STREPTOCOCCAL PROTEIN G (C2 FRAGMENT)



T1	T2	Y3	K4	L5	V6	I7	I8	G9	L12	K13	T16	T17	T18	E19	A20	V21	D22	A23	A24	T25	A26	E27	K28	V29	F30	K31	A34	N35	V39	D40	W43	T44	Y45	D46	D47	A48	T49	K50	T51	F52	T53	V54	T55	E56
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.60Å 110.60Å 160.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 18.35 – 3.20	Depositor EDS
% Data completeness (in resolution range)	72.0 (8.00-3.20) 72.7 (18.35-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.289 , 0.357 0.294 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.0	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 58.6	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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.

## 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	0.80	1/1702 (0.1%)	0.94	1/2316 (0.0%)
1	B	0.81	1/1702 (0.1%)	0.94	1/2316 (0.0%)
2	C	0.73	0/440	0.92	0/597
2	D	0.73	0/440	0.92	0/597
All	All	0.79	2/4284 (0.0%)	0.94	2/5826 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	GLU	CG-CD	5.22	1.59	1.51
1	A	293	GLU	CG-CD	5.20	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	LYS	N-CA-C	-8.45	88.18	111.00
1	A	288	LYS	N-CA-C	-8.44	88.20	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	1656	0	1630	161	1
1	B	1656	0	1630	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	434	0	415	39	1
2	D	434	0	415	40	0
All	All	4180	0	4090	368	2

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 44.

All (368) 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:A:357:GLU:HG3	1:B:349:TYR:CZ	1.85	1.10
1:A:371:GLY:HA2	1:A:403:SER:OG	1.73	0.89
1:A:357:GLU:HG3	1:B:349:TYR:OH	1.72	0.89
1:B:371:GLY:HA2	1:B:403:SER:OG	1.73	0.87
1:B:375:SER:HB3	1:B:404:PHE:CZ	2.10	0.86
1:A:375:SER:HB3	1:A:404:PHE:CZ	2.10	0.86
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.57	0.86
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.57	0.85
1:B:338:LYS:HD2	1:B:339:ALA:O	1.77	0.85
1:B:346:PRO:HD3	1:B:429:HIS:HD2	1.42	0.84
1:A:357:GLU:CG	1:B:349:TYR:CZ	2.59	0.84
1:A:338:LYS:HD2	1:A:339:ALA:O	1.77	0.84
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.13	0.84
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.13	0.84
1:A:346:PRO:HD3	1:A:429:HIS:HD2	1.42	0.83
2:C:7:ILE:HA	2:C:54:VAL:HG23	1.62	0.82
2:D:31:LYS:HG3	2:D:43:TRP:CZ2	2.16	0.81
2:D:7:ILE:HA	2:D:54:VAL:HG23	1.61	0.81
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.64	0.80
1:A:357:GLU:HB2	1:B:349:TYR:CE1	2.16	0.80
2:C:31:LYS:HG3	2:C:43:TRP:CZ2	2.16	0.80
1:B:261:CYS:HB2	1:B:277:TRP:HZ2	1.45	0.80
2:D:44:THR:OG1	2:D:53:THR:HB	1.82	0.79
2:C:44:THR:OG1	2:C:53:THR:HB	1.82	0.79
1:A:261:CYS:HB2	1:A:277:TRP:HZ2	1.45	0.79
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.19	0.78
1:A:437:THR:HG22	1:A:438:GLN:H	1.49	0.78
2:C:3:TYR:CE2	2:C:23:ALA:HA	2.20	0.77
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.64	0.77
2:D:3:TYR:CE2	2:D:23:ALA:HA	2.20	0.77
1:B:284:VAL:HB	1:B:287:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:THR:HG22	1:B:438:GLN:H	1.49	0.76
2:C:5:LEU:HD11	2:C:54:VAL:HG22	1.67	0.76
2:D:5:LEU:HD12	2:D:6:VAL:H	1.50	0.75
1:A:242:LEU:HD23	1:A:336:ILE:HB	1.69	0.75
2:C:18:THR:HG21	2:C:29:VAL:HG11	1.69	0.75
1:A:284:VAL:HB	1:A:287:ALA:HB2	1.67	0.75
1:B:377:ILE:HG12	1:B:378:ALA:N	2.02	0.74
2:D:5:LEU:HD11	2:D:54:VAL:HG22	1.67	0.74
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.69	0.74
1:B:257:PRO:HD3	1:B:310:HIS:NE2	2.03	0.73
2:C:5:LEU:HD12	2:C:6:VAL:H	1.51	0.73
1:A:377:ILE:HG12	1:A:378:ALA:N	2.02	0.73
2:D:18:THR:HG21	2:D:29:VAL:HG11	1.68	0.73
1:A:257:PRO:HD3	1:A:310:HIS:NE2	2.03	0.73
1:B:393:THR:HG23	1:B:408:SER:CB	2.19	0.72
2:C:45:TYR:O	2:C:46:ASP:HB2	1.89	0.72
2:D:45:TYR:O	2:D:46:ASP:HB2	1.89	0.72
1:B:375:SER:HB3	1:B:404:PHE:CE2	2.25	0.72
1:A:393:THR:HG23	1:A:408:SER:CB	2.19	0.71
1:A:375:SER:HB3	1:A:404:PHE:CE2	2.25	0.71
1:A:409:LYS:HE3	1:B:405:PHE:CD2	2.25	0.71
1:A:308:VAL:HG12	1:A:309:LEU:N	2.07	0.70
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.74	0.70
1:B:308:VAL:HG12	1:B:309:LEU:H	1.57	0.69
1:A:245:PRO:HD2	1:A:313:TRP:CH2	2.28	0.69
1:B:245:PRO:HD2	1:B:313:TRP:CH2	2.28	0.69
1:B:308:VAL:HG12	1:B:309:LEU:N	2.07	0.69
2:C:5:LEU:HD12	2:C:6:VAL:N	2.07	0.69
1:A:357:GLU:CB	1:B:349:TYR:CZ	2.75	0.69
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.73	0.68
1:A:277:TRP:CE3	1:A:306:LEU:HD23	2.29	0.68
2:D:5:LEU:HD12	2:D:6:VAL:N	2.07	0.68
1:A:308:VAL:HG13	1:A:319:TYR:CZ	2.29	0.68
1:A:357:GLU:HB2	1:B:349:TYR:CZ	2.30	0.67
1:A:351:LEU:HD12	1:B:351:LEU:HD12	1.75	0.67
1:B:277:TRP:CE3	1:B:306:LEU:HD23	2.29	0.67
1:B:296:TYR:OH	1:B:301:ARG:HB3	1.95	0.67
1:B:346:PRO:HD3	1:B:429:HIS:CD2	2.29	0.67
1:A:295:GLN:HB2	1:A:300:TYR:HE1	1.60	0.67
1:A:296:TYR:OH	1:A:301:ARG:HB3	1.95	0.67
1:B:308:VAL:HG13	1:B:319:TYR:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:OE2	1:B:439:LYS:HE3	1.95	0.67
1:A:346:PRO:HD3	1:A:429:HIS:CD2	2.29	0.66
1:B:290:LYS:O	1:B:304:SER:HA	1.95	0.66
1:A:290:LYS:O	1:A:304:SER:HA	1.95	0.66
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.76	0.66
1:A:357:GLU:CG	1:B:349:TYR:CE2	2.78	0.66
1:A:308:VAL:HG12	1:A:309:LEU:H	1.57	0.66
1:A:360:LYS:HE3	1:B:347:GLN:OE1	1.96	0.66
1:B:352:PRO:HB2	1:B:353:PRO:HD2	1.78	0.66
1:B:295:GLN:HB2	1:B:300:TYR:HE1	1.60	0.66
1:B:291:PRO:HA	1:B:303:VAL:O	1.97	0.65
2:C:5:LEU:HD22	2:C:30:PHE:HB3	1.77	0.65
1:B:430:GLU:HA	1:B:435:HIS:CD2	2.31	0.65
1:A:430:GLU:HA	1:A:435:HIS:CD2	2.32	0.65
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.76	0.65
1:A:352:PRO:HB2	1:A:353:PRO:HD2	1.77	0.65
1:A:357:GLU:CB	1:B:349:TYR:CE1	2.80	0.65
2:D:5:LEU:HD22	2:D:30:PHE:HB3	1.78	0.65
1:A:291:PRO:HA	1:A:303:VAL:O	1.97	0.64
1:A:245:PRO:HD2	1:A:313:TRP:CZ2	2.33	0.64
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.78	0.64
1:B:440:SER:O	1:B:441:LEU:HB2	1.96	0.64
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.79	0.64
1:A:397:VAL:HB	1:A:405:PHE:CE1	2.34	0.63
1:A:440:SER:O	1:A:441:LEU:HB2	1.96	0.63
1:B:397:VAL:HB	1:B:405:PHE:CE1	2.34	0.63
1:B:245:PRO:HD2	1:B:313:TRP:CZ2	2.33	0.63
1:B:279:VAL:HG23	1:B:284:VAL:HG21	1.80	0.63
1:B:393:THR:HG23	1:B:408:SER:HB2	1.81	0.63
1:A:393:THR:HG23	1:A:408:SER:HB2	1.81	0.63
1:A:279:VAL:HG23	1:A:284:VAL:HG21	1.80	0.62
1:A:239:SER:O	1:A:264:VAL:HG22	1.99	0.62
1:B:239:SER:O	1:B:264:VAL:HG22	1.99	0.62
1:B:429:HIS:ND1	1:B:430:GLU:N	2.48	0.61
2:C:3:TYR:CD2	2:C:26:ALA:HB2	2.36	0.61
1:A:357:GLU:HB2	1:B:349:TYR:CD1	2.34	0.61
2:D:3:TYR:CD2	2:D:26:ALA:HB2	2.36	0.60
1:A:429:HIS:ND1	1:A:430:GLU:N	2.48	0.60
1:A:257:PRO:HD3	1:A:310:HIS:CD2	2.38	0.59
2:D:16:THR:CG2	2:D:17:THR:N	2.66	0.59
1:B:414:LYS:HE3	1:B:418:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:HG23	1:B:408:SER:OG	2.03	0.59
1:B:257:PRO:HD3	1:B:310:HIS:CD2	2.37	0.58
2:C:16:THR:CG2	2:C:17:THR:N	2.66	0.58
1:A:393:THR:HG23	1:A:408:SER:OG	2.03	0.58
1:B:277:TRP:HE3	1:B:306:LEU:HD23	1.67	0.58
2:D:44:THR:O	2:D:52:PHE:HA	2.03	0.58
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.85	0.58
1:A:414:LYS:HE3	1:A:418:GLN:NE2	2.17	0.58
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.85	0.58
2:C:3:TYR:HD2	2:C:26:ALA:HB2	1.68	0.58
2:C:44:THR:O	2:C:52:PHE:HA	2.03	0.58
1:B:437:THR:HG22	1:B:438:GLN:N	2.17	0.58
1:A:266:VAL:CG1	1:A:300:TYR:HB2	2.34	0.58
1:A:262:VAL:HG22	1:A:303:VAL:HG22	1.86	0.58
1:A:411:THR:HG22	1:A:412:VAL:N	2.19	0.58
1:B:262:VAL:HG22	1:B:303:VAL:HG22	1.86	0.58
1:B:411:THR:HG22	1:B:412:VAL:N	2.19	0.58
1:A:437:THR:HG22	1:A:438:GLN:N	2.17	0.57
1:B:267:SER:H	1:B:299:THR:HB	1.70	0.57
1:A:277:TRP:HE3	1:A:306:LEU:HD23	1.67	0.57
2:D:3:TYR:HD2	2:D:26:ALA:HB2	1.68	0.57
1:A:267:SER:H	1:A:299:THR:HB	1.70	0.57
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.87	0.57
1:A:259:VAL:HG23	1:A:308:VAL:CG2	2.33	0.57
1:B:266:VAL:CG1	1:B:300:TYR:HB2	2.34	0.57
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.87	0.56
2:C:39:VAL:HA	2:C:56:GLU:OE2	2.06	0.56
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.33	0.55
1:B:283:GLN:NE2	1:B:285:HIS:HD2	2.04	0.55
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.89	0.55
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.89	0.55
1:A:277:TRP:HA	1:A:320:LYS:O	2.07	0.55
1:A:373:TYR:CG	1:A:374:PRO:HA	2.42	0.55
1:B:373:TYR:CG	1:B:374:PRO:HA	2.41	0.55
1:A:283:GLN:NE2	1:A:285:HIS:HD2	2.04	0.55
1:B:295:GLN:HB2	1:B:300:TYR:CE1	2.42	0.55
2:D:39:VAL:HA	2:D:56:GLU:OE2	2.06	0.55
1:B:379:VAL:HG12	1:B:380:GLU:N	2.21	0.54
1:B:276:ASN:HB3	1:B:278:TYR:CE1	2.42	0.54
1:A:276:ASN:HB3	1:A:278:TYR:CE1	2.42	0.54
1:A:432:LEU:HD13	1:A:437:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:HG12	1:A:380:GLU:N	2.21	0.53
1:B:277:TRP:HA	1:B:320:LYS:O	2.07	0.53
1:B:432:LEU:HD13	1:B:437:THR:OG1	2.08	0.53
2:C:31:LYS:HA	2:C:43:TRP:CH2	2.43	0.53
1:B:261:CYS:CB	1:B:277:TRP:HZ2	2.19	0.53
2:C:27:GLU:O	2:C:31:LYS:HB2	2.09	0.53
1:A:295:GLN:HB2	1:A:300:TYR:CE1	2.42	0.53
2:D:27:GLU:O	2:D:31:LYS:HB2	2.08	0.53
1:A:409:LYS:CE	1:B:405:PHE:CD2	2.91	0.53
2:D:31:LYS:HA	2:D:43:TRP:CH2	2.43	0.53
1:B:264:VAL:O	1:B:265:ASP:HB2	2.09	0.53
1:B:372:PHE:CD1	1:B:404:PHE:HB2	2.44	0.53
1:A:261:CYS:CB	1:A:277:TRP:HZ2	2.19	0.52
1:A:372:PHE:CD1	1:A:404:PHE:HB2	2.44	0.52
1:B:345:GLU:HG3	1:B:432:LEU:HD23	1.91	0.52
1:A:264:VAL:O	1:A:265:ASP:HB2	2.09	0.52
1:A:244:PRO:HD3	1:A:336:ILE:HD11	1.92	0.52
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.91	0.52
1:B:244:PRO:HD3	1:B:336:ILE:HD11	1.92	0.52
1:B:377:ILE:HG12	1:B:378:ALA:H	1.72	0.51
1:A:434:ASN:ND2	2:C:35:ASN:OD1	2.44	0.51
1:A:389:ASN:O	1:A:391:TYR:N	2.44	0.51
2:C:40:ASP:O	2:C:56:GLU:HG2	2.11	0.51
1:A:273:VAL:CG1	1:A:323:VAL:HG13	2.41	0.51
1:A:278:TYR:CD2	1:A:283:GLN:HB2	2.46	0.51
2:D:40:ASP:O	2:D:56:GLU:HG2	2.11	0.51
2:D:25:THR:HG22	2:D:25:THR:O	2.11	0.51
1:A:279:VAL:HG23	1:A:284:VAL:CG2	2.41	0.51
1:B:273:VAL:CG1	1:B:323:VAL:HG13	2.41	0.51
1:A:354:SER:HB2	1:B:349:TYR:HB3	1.92	0.51
1:B:411:THR:CG2	1:B:412:VAL:N	2.74	0.51
1:B:243:PHE:HD2	1:B:260:THR:HG22	1.76	0.51
1:B:270:ASP:HB3	1:B:325:ASN:HD21	1.76	0.50
1:A:266:VAL:HB	1:A:300:TYR:CB	2.42	0.50
1:A:277:TRP:CE3	1:A:306:LEU:CD2	2.94	0.50
1:B:266:VAL:HB	1:B:300:TYR:CA	2.41	0.50
1:B:279:VAL:HG23	1:B:284:VAL:CG2	2.41	0.50
1:B:406:LEU:C	1:B:406:LEU:HD12	2.32	0.50
1:A:246:LYS:HB2	1:A:249:ASP:OD2	2.11	0.50
1:A:320:LYS:HE2	1:A:333:GLU:HG2	1.93	0.50
1:A:406:LEU:HD12	1:A:406:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HB	1:A:300:TYR:CA	2.41	0.50
1:B:266:VAL:HB	1:B:300:TYR:CB	2.42	0.50
1:B:277:TRP:CE3	1:B:306:LEU:CD2	2.94	0.50
1:B:278:TYR:CD2	1:B:283:GLN:HB2	2.46	0.50
1:A:411:THR:CG2	1:A:412:VAL:N	2.74	0.50
1:B:389:ASN:O	1:B:391:TYR:N	2.44	0.50
1:A:283:GLN:NE2	1:A:285:HIS:CD2	2.79	0.50
1:A:362:GLN:HA	1:A:412:VAL:O	2.12	0.50
1:A:394:THR:HG22	1:B:397:VAL:HG21	1.94	0.50
1:B:246:LYS:HB2	1:B:249:ASP:OD2	2.11	0.50
1:B:296:TYR:OH	1:B:301:ARG:HD3	2.12	0.50
1:B:273:VAL:HG13	1:B:323:VAL:HG13	1.93	0.50
1:A:296:TYR:O	1:A:297:ASN:HB3	2.11	0.50
1:B:434:ASN:ND2	2:D:35:ASN:OD1	2.44	0.50
1:B:283:GLN:NE2	1:B:285:HIS:CD2	2.79	0.50
2:C:25:THR:O	2:C:25:THR:HG22	2.11	0.50
1:A:286:ASN:O	1:A:288:LYS:N	2.45	0.49
1:B:296:TYR:O	1:B:297:ASN:HB3	2.11	0.49
1:A:270:ASP:HB3	1:A:325:ASN:HD21	1.76	0.49
1:A:296:TYR:OH	1:A:301:ARG:HD3	2.12	0.49
1:B:320:LYS:HE2	1:B:333:GLU:HG2	1.93	0.49
1:A:377:ILE:HG12	1:A:378:ALA:H	1.72	0.49
1:B:362:GLN:HA	1:B:412:VAL:O	2.12	0.49
2:D:3:TYR:HD1	2:D:50:LYS:HB3	1.77	0.49
1:A:243:PHE:HD2	1:A:260:THR:HG22	1.76	0.49
1:A:273:VAL:HG13	1:A:323:VAL:HG13	1.93	0.49
1:A:345:GLU:HA	1:A:431:ALA:CB	2.43	0.49
2:C:12:LEU:HD12	2:C:13:LYS:N	2.27	0.49
1:A:276:ASN:CB	1:A:322:LYS:HB3	2.42	0.49
1:A:371:GLY:HA2	1:A:403:SER:CB	2.43	0.49
1:B:345:GLU:HA	1:B:431:ALA:CB	2.43	0.49
1:A:356:GLU:CD	1:B:439:LYS:HE3	2.33	0.49
1:A:356:GLU:HB2	1:B:439:LYS:HZ1	1.77	0.49
1:B:371:GLY:HA2	1:B:403:SER:CB	2.43	0.49
2:C:3:TYR:HD1	2:C:50:LYS:HB3	1.77	0.49
1:A:308:VAL:CG1	1:A:309:LEU:H	2.25	0.48
1:B:286:ASN:O	1:B:288:LYS:N	2.45	0.48
1:A:351:LEU:CD1	1:B:351:LEU:HD12	2.41	0.48
1:B:312:ASN:HB3	1:B:317:LYS:HG3	1.95	0.48
1:B:410:LEU:HG	1:B:411:THR:N	2.22	0.48
1:A:377:ILE:CG1	1:A:378:ALA:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:ALA:O	2:C:26:ALA:HB3	2.14	0.48
2:D:51:THR:HG22	2:D:52:PHE:N	2.29	0.48
2:C:16:THR:HG23	2:C:17:THR:H	1.78	0.48
2:D:12:LEU:HD12	2:D:13:LYS:N	2.27	0.48
1:B:276:ASN:CB	1:B:322:LYS:HB3	2.42	0.48
1:A:357:GLU:CA	1:B:349:TYR:CE1	2.97	0.48
1:A:350:THR:C	1:A:351:LEU:HD23	2.34	0.48
1:B:377:ILE:CG1	1:B:378:ALA:N	2.75	0.48
1:B:397:VAL:HB	1:B:405:PHE:CD1	2.49	0.48
2:C:51:THR:HG22	2:C:52:PHE:N	2.29	0.48
2:D:16:THR:HG23	2:D:17:THR:H	1.78	0.48
1:B:308:VAL:CG1	1:B:309:LEU:H	2.25	0.47
1:A:345:GLU:HA	1:A:431:ALA:HB3	1.96	0.47
1:B:350:THR:C	1:B:351:LEU:HD23	2.34	0.47
1:A:397:VAL:HB	1:A:405:PHE:CD1	2.49	0.47
1:B:346:PRO:HB3	1:B:372:PHE:CB	2.44	0.47
1:A:272:GLN:O	1:A:325:ASN:HB2	2.14	0.47
1:B:272:GLN:O	1:B:325:ASN:HB2	2.14	0.47
2:D:23:ALA:O	2:D:26:ALA:HB3	2.14	0.47
1:A:312:ASN:HB3	1:A:317:LYS:HG3	1.95	0.47
1:A:436:TYR:CD1	1:A:437:THR:N	2.83	0.47
1:A:365:LEU:HD12	1:A:410:LEU:CD2	2.43	0.47
1:B:345:GLU:HA	1:B:431:ALA:HB3	1.96	0.47
1:A:346:PRO:HB3	1:A:372:PHE:CB	2.44	0.46
1:B:436:TYR:CD1	1:B:437:THR:N	2.83	0.46
2:D:2:THR:O	2:D:2:THR:HG22	2.15	0.46
2:C:31:LYS:O	2:C:34:ALA:HB3	2.16	0.46
1:B:308:VAL:CG1	1:B:309:LEU:N	2.76	0.46
2:D:6:VAL:O	2:D:54:VAL:HG23	2.16	0.46
2:C:12:LEU:HD12	2:C:12:LEU:C	2.36	0.46
1:A:286:ASN:C	1:A:288:LYS:N	2.69	0.46
1:A:308:VAL:CG1	1:A:309:LEU:N	2.76	0.46
1:B:365:LEU:HD12	1:B:410:LEU:CD2	2.44	0.46
2:D:31:LYS:O	2:D:34:ALA:HB3	2.16	0.46
2:D:9:GLY:HA2	2:D:56:GLU:HB2	1.98	0.46
1:B:286:ASN:C	1:B:288:LYS:N	2.69	0.46
1:A:288:LYS:C	1:A:289:THR:OG1	2.55	0.46
1:A:242:LEU:HD12	1:A:243:PHE:H	1.81	0.45
1:A:291:PRO:O	1:A:292:ARG:HB2	2.16	0.45
1:A:410:LEU:HG	1:A:411:THR:N	2.22	0.45
2:C:6:VAL:O	2:C:54:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:CE1	1:A:322:LYS:HD3	2.51	0.45
1:B:267:SER:OG	1:B:268:HIS:N	2.47	0.45
2:D:45:TYR:HA	2:D:51:THR:O	2.17	0.45
2:C:9:GLY:HA2	2:C:56:GLU:HB2	1.98	0.45
2:C:45:TYR:HA	2:C:51:THR:O	2.17	0.45
1:B:253:ILE:N	2:D:27:GLU:OE2	2.49	0.45
1:B:278:TYR:CE1	1:B:322:LYS:HD3	2.51	0.45
2:C:2:THR:HG22	2:C:2:THR:O	2.15	0.45
1:A:397:VAL:HG12	1:A:398:LEU:N	2.32	0.45
1:B:375:SER:HB3	1:B:404:PHE:CE1	2.50	0.45
1:A:357:GLU:HA	1:B:349:TYR:CE1	2.52	0.44
1:B:242:LEU:HD12	1:B:243:PHE:H	1.81	0.44
1:B:291:PRO:O	1:B:292:ARG:HB2	2.16	0.44
2:C:44:THR:HG1	2:C:53:THR:HB	1.82	0.44
2:D:12:LEU:C	2:D:12:LEU:HD12	2.36	0.44
1:A:351:LEU:HD12	1:B:351:LEU:CD1	2.44	0.44
1:B:433:HIS:O	1:B:434:ASN:HB2	2.16	0.44
1:B:314:LEU:HD21	1:B:435:HIS:NE2	2.32	0.44
1:A:291:PRO:O	1:A:292:ARG:CB	2.65	0.44
1:B:241:PHE:HE2	1:B:264:VAL:HG21	1.83	0.44
1:A:267:SER:OG	1:A:268:HIS:N	2.47	0.44
1:A:288:LYS:O	1:A:289:THR:OG1	2.33	0.44
1:B:266:VAL:CB	1:B:300:TYR:HB2	2.48	0.44
1:B:430:GLU:HA	1:B:435:HIS:HD2	1.83	0.44
1:B:266:VAL:HB	1:B:300:TYR:C	2.39	0.43
1:B:365:LEU:HD11	1:B:423:PHE:CD2	2.53	0.43
1:A:314:LEU:HD21	1:A:435:HIS:NE2	2.32	0.43
1:B:291:PRO:O	1:B:292:ARG:CB	2.65	0.43
1:A:375:SER:HB3	1:A:404:PHE:CE1	2.50	0.43
1:A:433:HIS:O	1:A:434:ASN:HB2	2.16	0.43
1:A:246:LYS:O	1:A:249:ASP:N	2.52	0.43
1:A:308:VAL:HG13	1:A:319:TYR:CE2	2.54	0.43
1:B:288:LYS:C	1:B:289:THR:OG1	2.55	0.43
1:B:308:VAL:HG13	1:B:319:TYR:CE2	2.54	0.43
1:A:365:LEU:HD11	1:A:423:PHE:CD2	2.53	0.43
1:A:266:VAL:HB	1:A:300:TYR:C	2.38	0.43
1:B:397:VAL:HG12	1:B:398:LEU:N	2.32	0.43
2:D:16:THR:HG23	2:D:17:THR:N	2.34	0.43
1:A:253:ILE:HG12	2:C:43:TRP:HB2	2.00	0.43
2:C:16:THR:HG23	2:C:17:THR:N	2.34	0.43
1:A:354:SER:CB	1:B:349:TYR:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:HE2	1:A:264:VAL:HG21	1.83	0.42
2:C:51:THR:HG22	2:C:52:PHE:H	1.84	0.42
2:D:31:LYS:HG3	2:D:43:TRP:CH2	2.53	0.42
1:B:253:ILE:HG12	2:D:43:TRP:HB2	2.00	0.42
1:A:253:ILE:N	1:A:253:ILE:HD12	2.34	0.42
1:A:266:VAL:CB	1:A:300:TYR:HB2	2.48	0.42
1:B:253:ILE:N	1:B:253:ILE:HD12	2.34	0.42
2:C:46:ASP:OD1	2:C:48:ALA:HB3	2.20	0.42
1:A:356:GLU:HB2	1:B:439:LYS:NZ	2.35	0.42
1:B:290:LYS:HA	1:B:291:PRO:HD3	1.76	0.42
2:C:31:LYS:HG3	2:C:43:TRP:CH2	2.53	0.42
1:A:277:TRP:HE3	1:A:306:LEU:CD2	2.31	0.42
2:D:46:ASP:OD1	2:D:48:ALA:HB3	2.20	0.42
1:A:349:TYR:CZ	1:B:357:GLU:HG3	2.55	0.42
1:B:436:TYR:CE1	1:B:437:THR:O	2.73	0.42
1:A:263:VAL:HG21	1:A:273:VAL:HG11	2.02	0.42
1:A:384:ASN:C	1:A:386:GLN:H	2.23	0.42
1:B:384:ASN:C	1:B:386:GLN:H	2.23	0.42
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.20	0.42
1:A:346:PRO:CD	1:A:429:HIS:HD2	2.23	0.42
1:B:263:VAL:HG21	1:B:273:VAL:HG11	2.02	0.42
1:B:253:ILE:O	1:B:310:HIS:HE1	2.03	0.41
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.47	0.41
2:D:43:TRP:HA	2:D:53:THR:O	2.21	0.41
2:D:44:THR:HG1	2:D:53:THR:HB	1.84	0.41
1:A:253:ILE:O	1:A:310:HIS:HE1	2.03	0.41
1:A:436:TYR:CE1	1:A:437:THR:O	2.73	0.41
1:B:277:TRP:HE3	1:B:306:LEU:CD2	2.31	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD12	1.79	0.41
1:A:278:TYR:HA	1:A:283:GLN:HA	2.02	0.41
1:A:312:ASN:OD1	1:A:317:LYS:HE3	2.21	0.41
2:C:22:ASP:OD1	2:C:22:ASP:N	2.50	0.41
1:A:312:ASN:CB	1:A:317:LYS:HG3	2.51	0.41
1:B:288:LYS:O	1:B:289:THR:OG1	2.33	0.41
1:B:312:ASN:OD1	1:B:317:LYS:HE3	2.21	0.41
2:D:22:ASP:OD1	2:D:22:ASP:N	2.50	0.41
1:A:278:TYR:OH	1:A:322:LYS:HD3	2.21	0.41
1:B:325:ASN:OD1	1:B:327:ALA:HB3	2.21	0.41
1:A:325:ASN:OD1	1:A:327:ALA:HB3	2.21	0.41
1:B:246:LYS:O	1:B:249:ASP:N	2.52	0.41
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PRO:CD	1:B:429:HIS:HD2	2.23	0.40
1:A:290:LYS:HA	1:A:291:PRO:HD3	1.76	0.40
1:A:257:PRO:HG2	1:A:308:VAL:O	2.21	0.40
1:B:288:LYS:HB3	1:B:289:THR:H	1.70	0.40
1:B:257:PRO:HG2	1:B:308:VAL:O	2.21	0.40
1:A:412:VAL:HG11	1:A:423:PHE:CZ	2.57	0.40
1:B:278:TYR:OH	1:B:322:LYS:HD3	2.22	0.40
2:C:43:TRP:HA	2:C:53:THR:O	2.21	0.40
2:D:51:THR:HG22	2:D:52:PHE:H	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:OD1	1:A:361:ASN:ND2[5_544]	1.95	0.25
2:C:37:ASN:ND2	2:C:37:ASN:ND2[7_555]	2.18	0.02

## 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	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1	8
1	B	204/206 (99%)	171 (84%)	19 (9%)	14 (7%)	1	8
2	C	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	3	22
2	D	54/56 (96%)	45 (83%)	7 (13%)	2 (4%)	3	22
All	All	516/524 (98%)	432 (84%)	52 (10%)	32 (6%)	1	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	291	PRO
1	A	292	ARG
1	A	298	SER
2	C	46	ASP
1	B	288	LYS
1	B	291	PRO
1	B	292	ARG
1	B	298	SER
2	D	46	ASP
1	A	285	HIS
1	A	339	ALA
1	A	385	GLY
1	A	390	ASN
1	A	441	LEU
2	C	21	VAL
1	B	285	HIS
1	B	339	ALA
1	B	385	GLY
1	B	390	ASN
1	B	441	LEU
2	D	21	VAL
1	A	289	THR
1	B	289	THR
1	A	297	ASN
1	A	438	GLN
1	B	297	ASN
1	B	438	GLN
1	A	287	ALA
1	B	287	ALA
1	A	247	PRO
1	B	247	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/193 (100%)	175 (91%)	18 (9%)	9	33
1	B	193/193 (100%)	175 (91%)	18 (9%)	9	33
2	C	46/46 (100%)	42 (91%)	4 (9%)	10	37
2	D	46/46 (100%)	42 (91%)	4 (9%)	10	37
All	All	478/478 (100%)	434 (91%)	44 (9%)	9	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	267	SER
1	A	288	LYS
1	A	289	THR
1	A	296	TYR
1	A	305	VAL
1	A	314	LEU
1	A	315	ASP
1	A	325	ASN
1	A	326	LYS
1	A	338	LYS
1	A	351	LEU
1	A	361	ASN
1	A	390	ASN
1	A	393	THR
1	A	405	PHE
1	A	410	LEU
1	A	440	SER
2	C	19	GLU
2	C	22	ASP
2	C	31	LYS
2	C	54	VAL
1	B	256	THR
1	B	267	SER
1	B	288	LYS
1	B	289	THR
1	B	296	TYR
1	B	305	VAL
1	B	314	LEU
1	B	315	ASP
1	B	325	ASN
1	B	326	LYS
1	B	338	LYS

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Mol	Chain	Res	Type
1	B	351	LEU
1	B	361	ASN
1	B	390	ASN
1	B	393	THR
1	B	405	PHE
1	B	410	LEU
1	B	440	SER
2	D	19	GLU
2	D	22	ASP
2	D	31	LYS
2	D	54	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	283	GLN
1	A	285	HIS
1	A	286	ASN
1	A	310	HIS
1	A	311	GLN
1	A	390	ASN
1	A	418	GLN
2	C	32	GLN
1	B	276	ASN
1	B	283	GLN
1	B	285	HIS
1	B	286	ASN
1	B	310	HIS
1	B	311	GLN
1	B	390	ASN
1	B	418	GLN
2	D	32	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](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	206/206 (100%)	-0.20	1 (0%) 91 86	2, 37, 83, 125	0
1	B	206/206 (100%)	0.31	18 (8%) 10 5	2, 37, 83, 125	0
2	C	56/56 (100%)	-0.01	0 100 100	2, 39, 73, 86	0
2	D	56/56 (100%)	-0.01	0 100 100	2, 39, 73, 86	0
All	All	524/524 (100%)	0.04	19 (3%) 42 27	2, 38, 83, 125	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	SER	6.8
1	B	239	SER	5.9
1	B	238	PRO	4.8
1	B	330	ALA	3.9
1	B	329	PRO	3.6
1	B	331	PRO	3.5
1	B	271	PRO	3.5
1	B	297	ASN	3.4
1	B	272	GLN	3.1
1	B	264	VAL	2.9
1	B	286	ASN	2.8
1	B	321	CYS	2.6
1	B	267	SER	2.4
1	B	288	LYS	2.3
1	B	287	ALA	2.2
1	B	276	ASN	2.1
1	B	325	ASN	2.1
1	B	301	ARG	2.1
1	A	292	ARG	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.