



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 2FFH / pdb\_00002ffh  
Title : THE SIGNAL SEQUENCE BINDING PROTEIN FFH FROM THERMUS  
AQUATICUS  
Authors : Keenan, R.J.; Freymann, D.M.; Walter, P.; Stroud, R.M.  
Deposited on : 1999-06-29  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

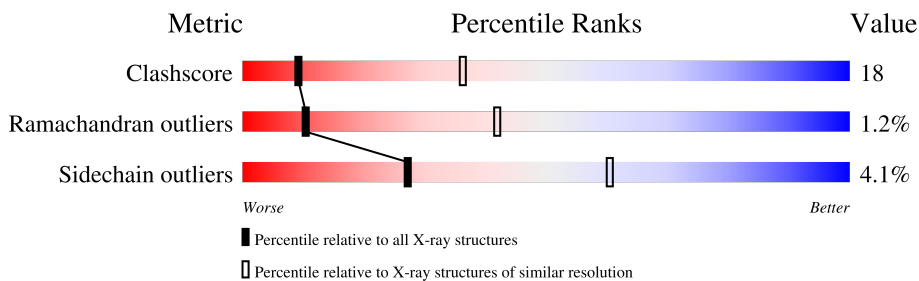
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (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 of 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	425	58% (Green) 35% (Yellow) . . (Grey)
1	B	425	60% (Green) 32% (Yellow) . . (Grey)
1	C	425	61% (Green) 33% (Yellow) . . (Grey)

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9484 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 PROTEIN (FFH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3151	1982	573	586	10	0	0	0
1	B	407	3151	1982	573	586	10	0	0	0
1	C	407	3151	1982	573	586	10	0	0	0

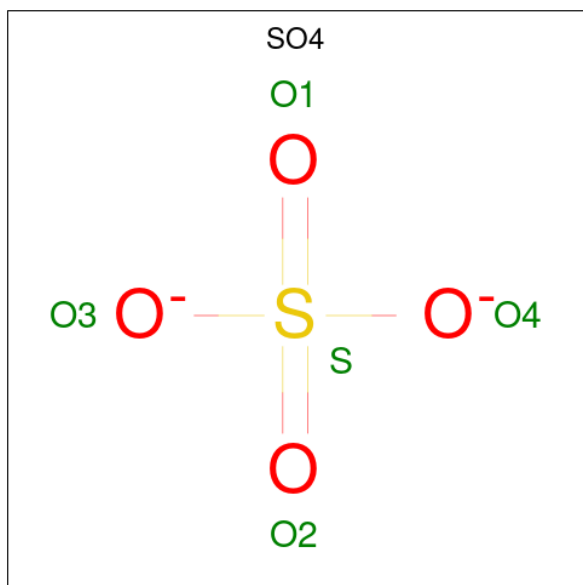
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	THR	ALA	SEE REMARK 999	UNP O07347
B	48	THR	ALA	SEE REMARK 999	UNP O07347
C	48	THR	ALA	SEE REMARK 999	UNP O07347

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cd	0	0
			5	5		
2	B	4	Total	Cd	0	0
			4	4		
2	C	7	Total	Cd	0	0
			7	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



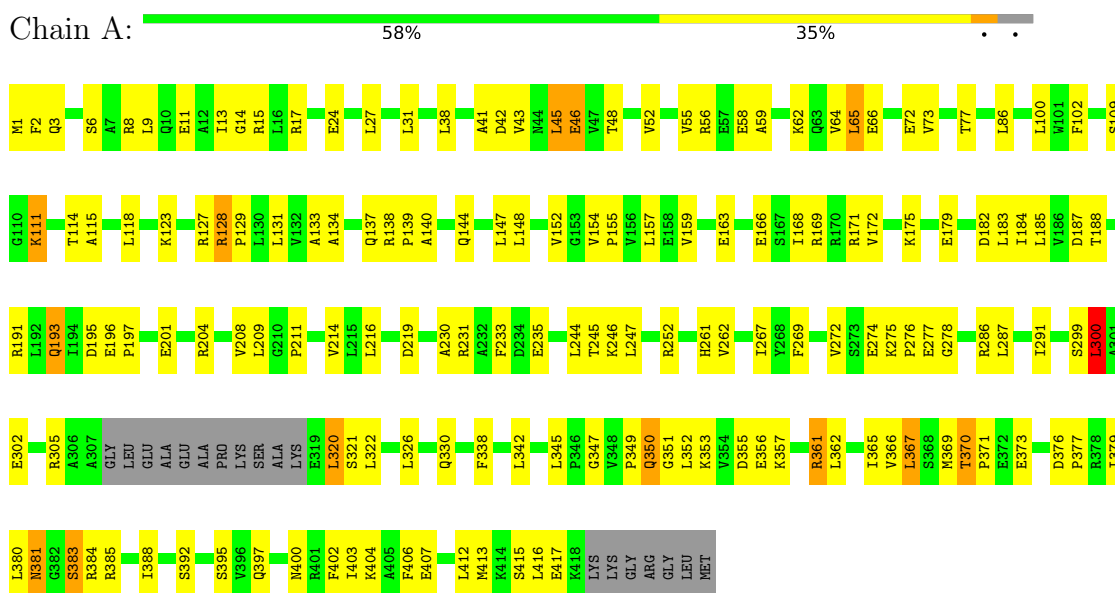
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

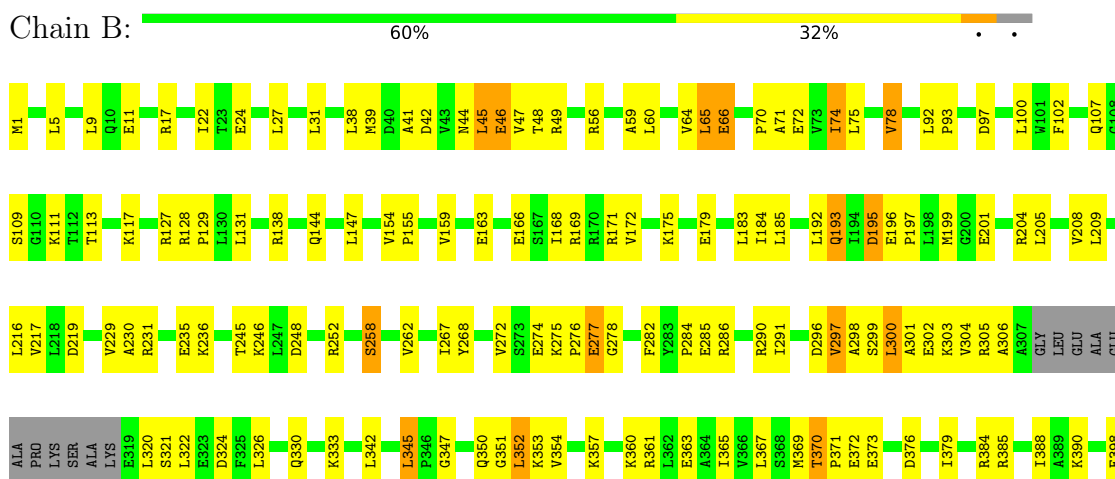
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: PROTEIN (FFH)



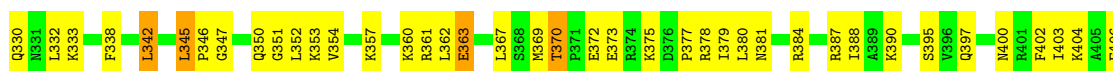
- Molecule 1: PROTEIN (FFH)





● Molecule 1: PROTEIN (FFH)

Chain C: 61% 33%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.05Å 195.05Å 335.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20	Depositor
% Data completeness (in resolution range)	90.4 (30.00-3.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.257 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

## 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: CD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.72	0/3184	1.08	13/4276 (0.3%)
1	B	0.81	2/3184 (0.1%)	1.10	15/4276 (0.4%)
1	C	0.83	2/3184 (0.1%)	1.10	11/4276 (0.3%)
All	All	0.79	4/9552 (0.0%)	1.09	39/12828 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	39	MET	SD-CE	5.85	1.94	1.79
1	C	294	MET	SD-CE	-5.81	1.65	1.79
1	B	199	MET	SD-CE	-5.81	1.65	1.79
1	C	199	MET	SD-CE	-5.45	1.66	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	LYS	N-CA-C	-10.25	100.04	112.54
1	B	353	LYS	N-CA-C	-9.46	101.00	112.54
1	C	353	LYS	N-CA-C	-9.33	101.16	112.54
1	A	45	LEU	N-CA-C	8.53	120.50	111.03
1	B	208	VAL	N-CA-C	8.19	118.12	110.42
1	C	208	VAL	N-CA-C	7.98	117.92	110.42
1	B	109	SER	N-CA-C	-7.39	103.39	113.30
1	B	128	ARG	CA-C-N	7.04	127.60	120.14
1	B	128	ARG	C-N-CA	7.04	127.60	120.14
1	A	8	ARG	N-CA-C	6.98	118.97	111.36
1	A	128	ARG	CA-C-N	6.85	126.77	119.85
1	A	128	ARG	C-N-CA	6.85	126.77	119.85
1	C	128	ARG	CA-C-N	6.84	126.76	119.85
1	C	128	ARG	C-N-CA	6.84	126.76	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ALA	N-CA-C	6.64	120.37	112.93
1	C	3	GLN	N-CA-C	6.59	119.02	111.11
1	A	208	VAL	N-CA-C	6.58	116.61	110.42
1	A	262	VAL	N-CA-C	6.51	116.67	110.42
1	B	296	ASP	N-CA-C	-6.47	100.94	110.52
1	A	233	PHE	N-CA-C	6.43	118.29	111.28
1	C	11	GLU	N-CA-C	-6.34	103.66	111.33
1	B	342	LEU	N-CA-C	-6.26	105.64	113.28
1	C	134	ALA	N-CA-C	6.09	119.75	112.93
1	A	123	LYS	N-CA-C	-6.03	104.78	111.36
1	B	229	VAL	N-CA-C	-5.92	104.74	110.72
1	A	392	SER	N-CA-C	5.91	117.52	111.14
1	B	277	GLU	N-CA-C	-5.65	105.58	113.37
1	B	306	ALA	N-CA-C	-5.62	106.26	113.23
1	B	74	ILE	N-CA-C	-5.47	105.19	110.72
1	B	236	LYS	N-CA-C	5.33	120.65	113.72
1	B	78	VAL	N-CA-C	-5.31	105.35	110.72
1	C	282	PHE	N-CA-C	5.27	117.82	109.96
1	C	363	GLU	N-CA-C	-5.27	105.65	111.71
1	A	361	ARG	N-CA-C	-5.27	105.62	111.36
1	A	109	SER	N-CA-C	-5.24	105.75	113.61
1	B	11	GLU	N-CA-C	-5.21	105.03	111.33
1	B	97	ASP	N-CA-C	-5.21	106.08	112.90
1	C	342	LEU	N-CA-C	-5.06	107.11	113.28
1	C	296	ASP	N-CA-C	-5.04	102.31	110.32

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3151	0	3319	133	0
1	B	3151	0	3319	124	1
1	C	3151	0	3319	117	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
2	C	7	0	0	0	1
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
All	All	9484	0	9957	354	1

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 18.

All (354) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:HB1	1:B:64:VAL:HG21	1.37	1.00
1:A:17:ARG:HH21	1:A:72:GLU:HG2	1.23	0.99
1:A:59:ALA:HB1	1:A:64:VAL:HG21	1.50	0.94
1:B:196:GLU:HG2	1:B:390:LYS:HE3	1.50	0.93
1:C:17:ARG:HH21	1:C:72:GLU:HG2	1.33	0.91
1:C:59:ALA:HB1	1:C:64:VAL:HG21	1.52	0.89
1:B:59:ALA:O	1:B:64:VAL:HG23	1.74	0.88
1:B:38:LEU:HD12	1:B:48:THR:HG23	1.59	0.84
1:C:59:ALA:O	1:C:64:VAL:HG23	1.76	0.83
1:C:369:MET:HG2	1:C:388:ILE:HD13	1.60	0.82
1:A:369:MET:HG2	1:A:388:ILE:HD13	1.63	0.79
1:A:361:ARG:O	1:A:365:ILE:HG13	1.83	0.79
1:C:168:ILE:O	1:C:172:VAL:HG23	1.83	0.78
1:A:300:LEU:HD13	1:B:300:LEU:HD22	1.64	0.77
1:A:59:ALA:O	1:A:64:VAL:HG23	1.86	0.76
1:B:175:LYS:HE3	1:B:179:GLU:OE2	1.87	0.75
1:B:1:MET:HE2	1:B:1:MET:HA	1.69	0.74
1:B:300:LEU:O	1:B:304:VAL:HG23	1.88	0.74
1:A:147:LEU:HD12	1:B:286:ARG:HG2	1.71	0.72
1:A:111:LYS:HE2	1:A:187:ASP:OD1	1.89	0.72
1:C:350:GLN:C	1:C:352:LEU:H	1.98	0.71
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.55	0.71
1:B:144:GLN:OE1	1:C:286:ARG:HD2	1.91	0.71
1:A:350:GLN:C	1:A:352:LEU:H	1.99	0.70
1:A:350:GLN:O	1:A:352:LEU:N	2.23	0.70
1:A:24:GLU:HA	1:A:65:LEU:HD21	1.72	0.70
1:A:100:LEU:HD12	1:A:184:ILE:HB	1.74	0.70
1:B:370:THR:HB	1:B:373:GLU:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HG2	1:C:275:LYS:HD3	1.74	0.69
1:B:369:MET:HG2	1:B:388:ILE:HD13	1.73	0.68
1:A:17:ARG:NH2	1:A:72:GLU:HG2	2.05	0.68
1:A:286:ARG:HG2	1:C:147:LEU:HD12	1.76	0.67
1:C:350:GLN:O	1:C:352:LEU:N	2.25	0.67
1:B:17:ARG:HH21	1:B:72:GLU:HG2	1.60	0.67
1:A:286:ARG:HD2	1:C:144:GLN:OE1	1.95	0.66
1:B:168:ILE:O	1:B:172:VAL:HG23	1.95	0.66
1:B:100:LEU:HD12	1:B:184:ILE:HB	1.77	0.66
1:B:197:PRO:O	1:B:201:GLU:HG3	1.95	0.66
1:A:370:THR:HB	1:A:373:GLU:HG3	1.78	0.66
1:A:64:VAL:HG22	1:A:73:VAL:HG11	1.78	0.66
1:C:193:GLN:HG2	1:C:370:THR:HA	1.78	0.66
1:A:102:PHE:HB2	1:A:214:VAL:HG22	1.78	0.65
1:A:9:LEU:O	1:A:13:ILE:HG13	1.97	0.65
1:A:216:LEU:HD21	1:A:230:ALA:HA	1.79	0.64
1:B:147:LEU:HD11	1:C:285:GLU:HB2	1.80	0.63
1:C:175:LYS:HE3	1:C:179:GLU:OE2	1.98	0.63
1:A:154:VAL:HG13	1:A:155:PRO:HD2	1.80	0.63
1:B:219:ASP:OD1	1:B:246:LYS:HD3	1.98	0.63
1:A:326:LEU:HD22	1:A:366:VAL:HG21	1.81	0.62
1:C:55:VAL:HG13	1:C:77:THR:HG21	1.81	0.62
1:A:322:LEU:HD11	1:A:402:PHE:CE2	2.35	0.61
1:B:350:GLN:O	1:B:352:LEU:N	2.26	0.61
1:B:1:MET:HE1	1:B:248:ASP:HA	1.83	0.61
1:A:17:ARG:HH21	1:A:72:GLU:CG	2.06	0.60
1:B:231:ARG:O	1:B:235:GLU:HB2	2.01	0.60
1:B:370:THR:HG22	1:B:372:GLU:H	1.66	0.60
1:C:114:THR:O	1:C:118:LEU:HB2	2.01	0.60
1:C:64:VAL:HG22	1:C:73:VAL:HG11	1.83	0.60
1:A:55:VAL:HG13	1:A:77:THR:HG21	1.84	0.60
1:B:216:LEU:HD12	1:B:217:VAL:N	2.16	0.60
1:B:59:ALA:HB1	1:B:64:VAL:CG2	2.22	0.60
1:B:163:GLU:CD	1:B:171:ARG:HH12	2.09	0.60
1:B:350:GLN:C	1:B:352:LEU:H	2.09	0.60
1:A:377:PRO:O	1:A:380:LEU:HB2	2.02	0.59
1:B:376:ASP:O	1:B:379:ILE:HG12	2.01	0.59
1:C:55:VAL:HG13	1:C:77:THR:CG2	2.32	0.59
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.67	0.59
1:C:127:ARG:HD3	1:C:182:ASP:OD1	2.02	0.59
1:B:74:ILE:O	1:B:78:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLU:OE2	1:C:375:LYS:HE2	2.02	0.59
1:B:276:PRO:C	1:B:278:GLY:H	2.11	0.58
1:A:2:PHE:CD1	1:A:291:ILE:HD11	2.38	0.58
1:A:272:VAL:O	1:A:272:VAL:HG12	2.03	0.58
1:C:131:LEU:HD23	1:C:185:LEU:HB2	1.85	0.58
1:C:275:LYS:HB3	1:C:276:PRO:HD2	1.85	0.58
1:B:276:PRO:HG2	1:B:277:GLU:H	1.68	0.58
1:C:333:LYS:O	1:C:333:LYS:HD3	2.04	0.58
1:B:147:LEU:HD12	1:C:286:ARG:HG2	1.86	0.57
1:B:286:ARG:O	1:B:290:ARG:HG3	2.04	0.57
1:B:322:LEU:HD11	1:B:402:PHE:CE2	2.39	0.57
1:A:38:LEU:HD22	1:A:43:VAL:HG21	1.86	0.57
1:C:370:THR:HG22	1:C:373:GLU:H	1.69	0.57
1:B:300:LEU:HD13	1:C:300:LEU:HB3	1.87	0.57
1:A:231:ARG:O	1:A:235:GLU:HB2	2.04	0.57
1:B:252:ARG:HG2	1:B:252:ARG:HH11	1.68	0.57
1:B:46:GLU:HG3	1:B:46:GLU:O	2.02	0.56
1:A:193:GLN:HG2	1:A:370:THR:HA	1.87	0.56
1:B:258:SER:O	1:B:262:VAL:HG23	2.05	0.56
1:C:362:LEU:HD22	1:C:402:PHE:CD1	2.40	0.56
1:A:138:ARG:NH1	1:A:191:ARG:HH11	2.04	0.56
1:C:127:ARG:O	1:C:129:PRO:HD3	2.06	0.56
1:A:144:GLN:OE1	1:B:286:ARG:HD2	2.05	0.56
1:A:415:SER:C	1:A:417:GLU:H	2.14	0.55
1:C:338:PHE:O	1:C:342:LEU:HG	2.06	0.55
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.21	0.55
1:C:345:LEU:C	1:C:347:GLY:H	2.14	0.55
1:C:16:LEU:HD11	1:C:30:THR:OG1	2.06	0.55
1:C:75:LEU:HD12	1:C:75:LEU:O	2.07	0.55
1:B:38:LEU:CD1	1:B:48:THR:HG23	2.34	0.55
1:A:148:LEU:O	1:A:152:VAL:HG22	2.07	0.55
1:B:24:GLU:HA	1:B:65:LEU:HD21	1.89	0.54
1:B:345:LEU:C	1:B:347:GLY:H	2.15	0.54
1:C:219:ASP:OD1	1:C:246:LYS:HD3	2.07	0.54
1:A:137:GLN:O	1:A:139:PRO:HD3	2.08	0.54
1:C:1:MET:HE2	1:C:1:MET:HA	1.90	0.54
1:B:276:PRO:HG2	1:B:277:GLU:HG3	1.88	0.54
1:C:2:PHE:CD1	1:C:291:ILE:HD11	2.43	0.54
1:A:175:LYS:HE3	1:A:179:GLU:OE2	2.08	0.54
1:C:252:ARG:HH11	1:C:252:ARG:HG2	1.73	0.54
1:C:65:LEU:C	1:C:66:GLU:HG3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG22	1:A:77:THR:HG22	1.90	0.53
1:A:129:PRO:HA	1:A:183:LEU:O	2.09	0.53
1:A:370:THR:HB	1:A:373:GLU:CG	2.38	0.53
1:C:350:GLN:C	1:C:352:LEU:N	2.67	0.53
1:C:415:SER:C	1:C:417:GLU:H	2.16	0.53
1:A:362:LEU:HD22	1:A:402:PHE:CD1	2.43	0.53
1:B:59:ALA:C	1:B:64:VAL:HG23	2.32	0.53
1:A:299:SER:H	1:A:302:GLU:HB2	1.73	0.53
1:B:27:LEU:HD12	1:B:27:LEU:O	2.09	0.53
1:C:163:GLU:OE2	1:C:171:ARG:NH1	2.42	0.53
1:C:197:PRO:O	1:C:201:GLU:HG3	2.09	0.53
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.74	0.53
1:B:196:GLU:N	1:B:197:PRO:HD2	2.24	0.53
1:C:196:GLU:HG2	1:C:390:LYS:HE3	1.90	0.53
1:A:370:THR:HG23	1:A:371:PRO:HD2	1.91	0.52
1:B:300:LEU:CD1	1:C:300:LEU:HB3	2.40	0.52
1:C:102:PHE:CE1	1:C:211:PRO:HG3	2.44	0.52
1:A:171:ARG:HG3	1:A:171:ARG:HH11	1.74	0.52
1:B:75:LEU:HD12	1:B:75:LEU:O	2.10	0.52
1:B:92:LEU:O	1:B:93:PRO:C	2.53	0.52
1:B:17:ARG:HG2	1:B:71:ALA:CB	2.40	0.52
1:B:93:PRO:HD3	1:B:268:TYR:CG	2.45	0.52
1:C:163:GLU:CD	1:C:171:ARG:HH12	2.18	0.52
1:A:127:ARG:HD3	1:A:182:ASP:OD1	2.09	0.52
1:C:74:ILE:O	1:C:78:VAL:HG23	2.09	0.52
1:A:362:LEU:O	1:A:366:VAL:HG23	2.10	0.52
1:B:385:ARG:NE	1:B:400:ASN:HD22	2.08	0.52
1:A:376:ASP:O	1:A:379:ILE:HG12	2.09	0.52
1:A:326:LEU:O	1:A:330:GLN:HG3	2.10	0.51
1:A:1:MET:HA	1:A:1:MET:HE2	1.92	0.51
1:B:370:THR:HG23	1:B:371:PRO:HD2	1.93	0.51
1:A:14:GLY:O	1:A:17:ARG:HB2	2.11	0.51
1:C:111:LYS:HE2	1:C:187:ASP:OD1	2.11	0.51
1:C:107:GLN:HB3	1:C:192:LEU:HD23	1.93	0.50
1:A:11:GLU:HG2	1:A:15:ARG:NH1	2.27	0.50
1:A:27:LEU:O	1:A:31:LEU:HG	2.12	0.50
1:A:86:LEU:HD13	1:A:287:LEU:HD23	1.93	0.50
1:A:133:ALA:O	1:A:159:VAL:HG22	2.12	0.50
1:B:27:LEU:O	1:B:31:LEU:HG	2.12	0.50
1:B:370:THR:HB	1:B:373:GLU:CG	2.40	0.50
1:B:373:GLU:HA	1:B:379:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:HE3	1:C:188:THR:O	2.10	0.50
1:C:377:PRO:O	1:C:380:LEU:HB2	2.10	0.50
1:B:46:GLU:OE2	1:B:49:ARG:NH2	2.45	0.50
1:B:100:LEU:HD21	1:B:209:LEU:HB3	1.92	0.50
1:C:415:SER:O	1:C:417:GLU:N	2.45	0.50
1:A:118:LEU:HD11	1:A:269:PHE:CZ	2.45	0.50
1:A:370:THR:HB	1:A:373:GLU:CD	2.37	0.50
1:A:127:ARG:C	1:A:129:PRO:HD3	2.37	0.50
1:A:415:SER:O	1:A:417:GLU:N	2.45	0.50
1:B:193:GLN:HG2	1:B:370:THR:HA	1.94	0.50
1:A:64:VAL:HG22	1:A:73:VAL:CG1	2.42	0.49
1:A:385:ARG:NE	1:A:400:ASN:HD22	2.08	0.49
1:B:166:GLU:HB3	1:B:169:ARG:HH21	1.74	0.49
1:C:31:LEU:HD11	1:C:56:ARG:HB2	1.94	0.49
1:A:1:MET:O	1:A:2:PHE:C	2.54	0.49
1:A:41:ALA:O	1:A:42:ASP:HB2	2.12	0.49
1:A:196:GLU:N	1:A:197:PRO:HD2	2.27	0.49
1:B:248:ASP:HB3	1:B:272:VAL:O	2.12	0.49
1:B:361:ARG:O	1:B:365:ILE:HG13	2.11	0.49
1:C:59:ALA:C	1:C:64:VAL:HG23	2.37	0.49
1:C:96:LYS:NZ	1:C:212:ASP:OD1	2.46	0.49
1:A:163:GLU:CD	1:A:171:ARG:HH12	2.21	0.49
1:B:326:LEU:O	1:B:330:GLN:HG3	2.12	0.49
1:C:216:LEU:HD21	1:C:230:ALA:HA	1.94	0.49
1:A:168:ILE:O	1:A:172:VAL:HG23	2.13	0.49
1:B:65:LEU:C	1:B:66:GLU:HG3	2.38	0.49
1:B:131:LEU:HD23	1:B:185:LEU:HB2	1.95	0.49
1:C:59:ALA:HB1	1:C:64:VAL:CG2	2.34	0.49
1:A:127:ARG:O	1:A:129:PRO:HD3	2.12	0.49
1:A:2:PHE:HD1	1:A:291:ILE:HD11	1.78	0.49
1:A:128:ARG:NH1	1:A:179:GLU:O	2.42	0.49
1:B:345:LEU:N	1:B:345:LEU:HD12	2.27	0.49
1:C:159:VAL:HG11	1:C:168:ILE:HD13	1.94	0.49
1:A:140:ALA:O	1:A:144:GLN:HG2	2.14	0.48
1:A:299:SER:OG	1:A:302:GLU:HG3	2.13	0.48
1:A:27:LEU:O	1:A:27:LEU:HD12	2.13	0.48
1:A:3:GLN:OE1	1:A:305:ARG:HD2	2.13	0.48
1:A:154:VAL:CG1	1:A:155:PRO:HD2	2.43	0.48
1:A:350:GLN:C	1:A:352:LEU:N	2.66	0.48
1:C:352:LEU:C	1:C:354:VAL:N	2.71	0.48
1:C:46:GLU:OE2	1:C:49:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:H	1:B:302:GLU:CD	2.21	0.48
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.75	0.48
1:B:31:LEU:HD11	1:B:56:ARG:HB2	1.96	0.48
1:C:370:THR:HB	1:C:373:GLU:HG3	1.96	0.48
1:A:403:ILE:O	1:A:406:PHE:HB3	2.14	0.48
1:A:197:PRO:O	1:A:201:GLU:HG3	2.14	0.47
1:C:216:LEU:CD2	1:C:230:ALA:HA	2.44	0.47
1:A:380:LEU:HD23	1:A:384:ARG:HD3	1.96	0.47
1:B:113:THR:HG22	1:B:117:LYS:HE3	1.96	0.47
1:C:219:ASP:CG	1:C:246:LYS:HD3	2.38	0.47
1:C:345:LEU:O	1:C:347:GLY:N	2.45	0.47
1:B:41:ALA:O	1:B:42:ASP:HB2	2.13	0.47
1:A:345:LEU:C	1:A:347:GLY:H	2.22	0.47
1:C:36:ARG:O	1:C:37:ALA:C	2.56	0.47
1:A:31:LEU:HD11	1:A:56:ARG:HB2	1.95	0.47
1:A:219:ASP:OD1	1:A:219:ASP:C	2.57	0.47
1:C:395:SER:C	1:C:397:GLN:N	2.72	0.47
1:C:413:MET:HE3	1:C:413:MET:HA	1.97	0.47
1:A:275:LYS:HZ1	1:C:275:LYS:HZ3	1.63	0.47
1:B:64:VAL:C	1:B:66:GLU:H	2.23	0.47
1:C:299:SER:O	1:C:303:LYS:HG3	2.15	0.46
1:A:355:ASP:O	1:A:356:GLU:C	2.58	0.46
1:B:350:GLN:C	1:B:352:LEU:N	2.73	0.46
1:C:48:THR:O	1:C:52:VAL:HG23	2.16	0.46
1:A:58:GLU:O	1:A:62:LYS:HG2	2.15	0.46
1:A:131:LEU:HD23	1:A:185:LEU:HB2	1.98	0.46
1:A:277:GLU:OE1	1:C:276:PRO:HG3	2.16	0.46
1:A:373:GLU:HA	1:A:379:ILE:HD11	1.97	0.46
1:B:352:LEU:C	1:B:354:VAL:N	2.73	0.46
1:C:41:ALA:O	1:C:42:ASP:HB2	2.16	0.46
1:B:301:ALA:O	1:B:305:ARG:N	2.47	0.46
1:C:127:ARG:C	1:C:129:PRO:HD3	2.41	0.46
1:C:154:VAL:HG13	1:C:155:PRO:HD2	1.98	0.46
1:C:148:LEU:O	1:C:152:VAL:HG22	2.15	0.46
1:C:196:GLU:N	1:C:197:PRO:HD2	2.30	0.46
1:A:55:VAL:HG13	1:A:77:THR:CG2	2.45	0.46
1:B:333:LYS:HD3	1:B:333:LYS:O	2.16	0.46
1:C:370:THR:CG2	1:C:372:GLU:H	2.29	0.46
1:A:6:SER:OG	1:A:291:ILE:O	2.20	0.46
1:A:59:ALA:C	1:A:64:VAL:HG23	2.39	0.46
1:A:138:ARG:HD2	1:A:191:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:HD12	1:C:27:LEU:O	2.16	0.46
1:A:300:LEU:HD23	1:A:300:LEU:H	1.80	0.46
1:B:129:PRO:HA	1:B:183:LEU:O	2.15	0.46
1:B:354:VAL:HG23	1:B:354:VAL:O	2.16	0.46
1:A:114:THR:O	1:A:115:ALA:C	2.56	0.46
1:B:5:LEU:HD11	1:B:9:LEU:HD11	1.98	0.46
1:B:284:PRO:O	1:B:285:GLU:C	2.58	0.46
1:B:102:PHE:CE1	1:B:209:LEU:HD12	2.52	0.45
1:B:345:LEU:N	1:B:345:LEU:CD1	2.78	0.45
1:C:301:ALA:O	1:C:302:GLU:C	2.59	0.45
1:B:321:SER:OG	1:B:324:ASP:OD1	2.33	0.45
1:C:370:THR:HB	1:C:373:GLU:CD	2.41	0.45
1:B:245:THR:O	1:B:246:LYS:C	2.59	0.45
1:B:275:LYS:HB3	1:B:276:PRO:HD2	1.99	0.45
1:B:321:SER:O	1:B:324:ASP:N	2.49	0.45
1:C:171:ARG:HG3	1:C:171:ARG:NH1	2.31	0.45
1:A:216:LEU:CD2	1:A:230:ALA:HA	2.44	0.45
1:A:400:ASN:O	1:A:404:LYS:HG2	2.16	0.45
1:B:415:SER:C	1:B:417:GLU:H	2.24	0.45
1:C:360:LYS:HA	1:C:363:GLU:HB2	1.98	0.45
1:C:128:ARG:NH1	1:C:179:GLU:O	2.50	0.45
1:A:138:ARG:HD2	1:A:191:ARG:HH12	1.82	0.44
1:A:338:PHE:O	1:A:342:LEU:HG	2.17	0.44
1:B:166:GLU:CG	1:B:169:ARG:HH21	2.30	0.44
1:C:380:LEU:CD1	1:C:403:ILE:HD13	2.47	0.44
1:B:159:VAL:HG11	1:B:168:ILE:HD13	1.99	0.44
1:B:276:PRO:HG2	1:B:277:GLU:N	2.32	0.44
1:C:24:GLU:HA	1:C:65:LEU:HD21	2.00	0.44
1:C:160:MET:O	1:C:161:ASP:C	2.61	0.44
1:C:174:GLU:O	1:C:178:LEU:HG	2.18	0.44
1:A:349:PRO:O	1:A:350:GLN:HB2	2.18	0.44
1:A:380:LEU:CD1	1:A:403:ILE:HD13	2.48	0.44
1:A:415:SER:C	1:A:417:GLU:N	2.75	0.44
1:B:147:LEU:CD1	1:C:285:GLU:HB2	2.48	0.44
1:B:276:PRO:C	1:B:278:GLY:N	2.75	0.44
1:B:163:GLU:OE2	1:B:171:ARG:NH1	2.51	0.44
1:C:122:TYR:CD1	1:C:183:LEU:HD21	2.53	0.44
1:C:345:LEU:HD12	1:C:345:LEU:N	2.32	0.44
1:A:370:THR:HG22	1:A:373:GLU:H	1.82	0.43
1:B:357:LYS:O	1:B:361:ARG:HG2	2.18	0.43
1:C:2:PHE:O	1:C:6:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PRO:C	1:A:278:GLY:H	2.25	0.43
1:C:370:THR:HG22	1:C:372:GLU:H	1.82	0.43
1:A:64:VAL:CG2	1:A:73:VAL:HG11	2.47	0.43
1:B:154:VAL:HG13	1:B:155:PRO:HD2	1.99	0.43
1:C:140:ALA:O	1:C:144:GLN:HG2	2.18	0.43
1:A:274:GLU:OE2	1:B:297:VAL:HG12	2.17	0.43
1:A:111:LYS:NZ	1:A:111:LYS:HB3	2.34	0.43
1:C:36:ARG:O	1:C:39:MET:N	2.52	0.42
1:A:245:THR:O	1:A:246:LYS:C	2.60	0.42
1:B:102:PHE:HZ	1:B:205:LEU:HG	1.84	0.42
1:B:384:ARG:O	1:B:388:ILE:HG13	2.19	0.42
1:A:171:ARG:HG3	1:A:171:ARG:NH1	2.34	0.42
1:A:395:SER:C	1:A:397:GLN:N	2.74	0.42
1:A:65:LEU:C	1:A:66:GLU:HG3	2.44	0.42
1:A:245:THR:C	1:A:247:LEU:N	2.75	0.42
1:C:100:LEU:HD12	1:C:184:ILE:HB	2.01	0.42
1:A:219:ASP:CG	1:A:246:LYS:HD3	2.44	0.42
1:C:415:SER:C	1:C:417:GLU:N	2.78	0.42
1:A:244:LEU:CD1	1:A:267:ILE:HD13	2.49	0.42
1:A:275:LYS:NZ	1:C:275:LYS:NZ	2.68	0.42
1:B:44:ASN:CG	1:B:45:LEU:N	2.77	0.42
1:C:409:MET:O	1:C:413:MET:HB2	2.20	0.42
1:A:321:SER:O	1:A:322:LEU:C	2.61	0.42
1:B:360:LYS:HA	1:B:363:GLU:HB2	2.01	0.42
1:C:357:LYS:O	1:C:361:ARG:HG2	2.20	0.42
1:A:102:PHE:CE1	1:A:211:PRO:HG3	2.54	0.42
1:A:299:SER:O	1:A:300:LEU:C	2.63	0.42
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.91	0.42
1:C:378:ARG:C	1:C:380:LEU:N	2.78	0.42
1:A:166:GLU:HB3	1:A:169:ARG:HH21	1.84	0.42
1:B:291:ILE:O	1:B:291:ILE:HG22	2.20	0.42
1:C:64:VAL:CG2	1:C:73:VAL:HG11	2.49	0.42
1:B:404:LYS:HA	1:B:404:LYS:HD3	1.85	0.41
1:C:379:ILE:O	1:C:384:ARG:NH1	2.53	0.41
1:A:86:LEU:CD1	1:A:287:LEU:HD23	2.50	0.41
1:C:10:GLN:O	1:C:11:GLU:C	2.61	0.41
1:C:131:LEU:HB2	1:C:156:VAL:HG22	2.01	0.41
1:A:168:ILE:O	1:A:169:ARG:C	2.62	0.41
1:A:320:LEU:HD13	1:A:413:MET:HG2	2.02	0.41
1:B:44:ASN:HB3	1:B:47:VAL:CG2	2.50	0.41
1:B:193:GLN:HE21	1:B:193:GLN:HB2	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:SER:OG	1:C:302:GLU:HG3	2.21	0.41
1:A:46:GLU:HG2	1:A:261:HIS:CE1	2.55	0.41
1:A:169:ARG:HA	1:A:209:LEU:CD2	2.50	0.41
1:B:166:GLU:CB	1:B:169:ARG:HH21	2.33	0.41
1:B:195:ASP:OD1	1:B:195:ASP:N	2.53	0.41
1:B:345:LEU:C	1:B:347:GLY:N	2.79	0.41
1:A:406:PHE:O	1:A:407:GLU:C	2.63	0.41
1:B:107:GLN:HB3	1:B:192:LEU:HD23	2.02	0.41
1:C:384:ARG:HG2	1:C:387:ARG:HH12	1.86	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.88	0.41
1:B:138:ARG:NE	1:C:72:GLU:OE1	2.49	0.41
1:B:361:ARG:NH2	1:B:398:GLU:OE2	2.48	0.41
1:C:102:PHE:HZ	1:C:205:LEU:HG	1.86	0.41
1:C:326:LEU:O	1:C:330:GLN:HG3	2.20	0.41
1:C:345:LEU:C	1:C:347:GLY:N	2.79	0.41
1:A:31:LEU:CD1	1:A:56:ARG:HB2	2.51	0.41
1:B:267:ILE:HB	1:B:282:PHE:CD2	2.56	0.41
1:B:406:PHE:O	1:B:407:GLU:C	2.63	0.41
1:C:345:LEU:N	1:C:345:LEU:CD1	2.83	0.41
1:C:370:THR:HG22	1:C:372:GLU:N	2.36	0.41
1:A:48:THR:O	1:A:52:VAL:HG23	2.21	0.41
1:A:157:LEU:HD23	1:A:172:VAL:HG22	2.02	0.41
1:A:244:LEU:HD11	1:A:267:ILE:HD13	2.03	0.41
1:A:275:LYS:NZ	1:C:275:LYS:HZ3	2.19	0.41
1:A:381:ASN:ND2	1:A:383:SER:H	2.19	0.41
1:A:413:MET:HE3	1:A:413:MET:HA	2.02	0.41
1:A:357:LYS:O	1:A:361:ARG:HG2	2.20	0.41
1:B:22:ILE:HG23	1:B:70:PRO:HG3	2.03	0.41
1:B:246:LYS:HE3	1:C:298:ALA:HB2	2.02	0.41
1:B:252:ARG:HG2	1:B:252:ARG:NH1	2.35	0.41
1:B:298:ALA:HA	1:B:302:GLU:OE1	2.21	0.41
1:C:400:ASN:O	1:C:404:LYS:HG2	2.21	0.41
1:C:403:ILE:O	1:C:406:PHE:HB3	2.21	0.41
1:B:286:ARG:HD2	1:B:286:ARG:HA	1.75	0.40
1:B:219:ASP:CG	1:B:246:LYS:HD3	2.46	0.40
1:B:216:LEU:HD21	1:B:230:ALA:HA	2.02	0.40
1:A:138:ARG:NE	1:B:72:GLU:OE1	2.54	0.40
1:B:216:LEU:HD12	1:B:217:VAL:H	1.83	0.40
1:B:102:PHE:HE1	1:B:209:LEU:HD12	1.85	0.40

All (1) 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:B:169:ARG:CZ	2:C:705:CD:CD[3_665]	2.03	0.17

### 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	403/425 (95%)	358 (89%)	39 (10%)	6 (2%)	8	37
1	B	403/425 (95%)	370 (92%)	28 (7%)	5 (1%)	10	42
1	C	403/425 (95%)	370 (92%)	30 (7%)	3 (1%)	18	52
All	All	1209/1275 (95%)	1098 (91%)	97 (8%)	14 (1%)	10	42

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	LEU
1	C	416	LEU
1	B	127	ARG
1	B	351	GLY
1	C	351	GLY
1	A	188	THR
1	A	351	GLY
1	B	65	LEU
1	B	416	LEU
1	A	65	LEU
1	B	352	LEU
1	A	300	LEU
1	A	350	GLN
1	C	346	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	330/342 (96%)	317 (96%)	13 (4%)	28	62
1	B	330/342 (96%)	314 (95%)	16 (5%)	23	56
1	C	330/342 (96%)	318 (96%)	12 (4%)	31	63
All	All	990/1026 (96%)	949 (96%)	41 (4%)	27	60

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

Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	GLU
1	A	111	LYS
1	A	193	GLN
1	A	195	ASP
1	A	204	ARG
1	A	300	LEU
1	A	320	LEU
1	A	367	LEU
1	A	370	THR
1	A	381	ASN
1	A	383	SER
1	A	412	LEU
1	B	45	LEU
1	B	46	GLU
1	B	66	GLU
1	B	111	LYS
1	B	193	GLN
1	B	195	ASP
1	B	204	ARG
1	B	258	SER
1	B	274	GLU
1	B	297	VAL
1	B	300	LEU
1	B	303	LYS
1	B	320	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	345	LEU
1	B	367	LEU
1	B	370	THR
1	C	45	LEU
1	C	56	ARG
1	C	66	GLU
1	C	111	LYS
1	C	193	GLN
1	C	195	ASP
1	C	320	LEU
1	C	332	LEU
1	C	345	LEU
1	C	367	LEU
1	C	370	THR
1	C	381	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	331	ASN
1	A	381	ASN
1	A	400	ASN
1	B	193	GLN
1	B	331	ASN
1	B	381	ASN
1	B	400	ASN
1	C	3	GLN
1	C	4	GLN
1	C	63	GLN
1	C	193	GLN
1	C	224	GLN
1	C	261	HIS
1	C	331	ASN
1	C	381	ASN

### 5.3.3 RNA

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	C	770	-	4,4,4	0.52	0	6,6,6	0.35	0
3	SO4	A	750	-	4,4,4	0.31	0	6,6,6	0.20	0
3	SO4	B	760	-	4,4,4	0.36	0	6,6,6	0.53	0

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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.