



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:03 AM GMT

PDB ID : 1B6C  
Title : CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF THE  
TYPE I TGF-BETA RECEPTOR IN COMPLEX WITH FKBP12  
Authors : Huse, M.; Chen, Y.-G.; Massague, J.; Kuriyan, J.  
Deposited on : 1999-01-13  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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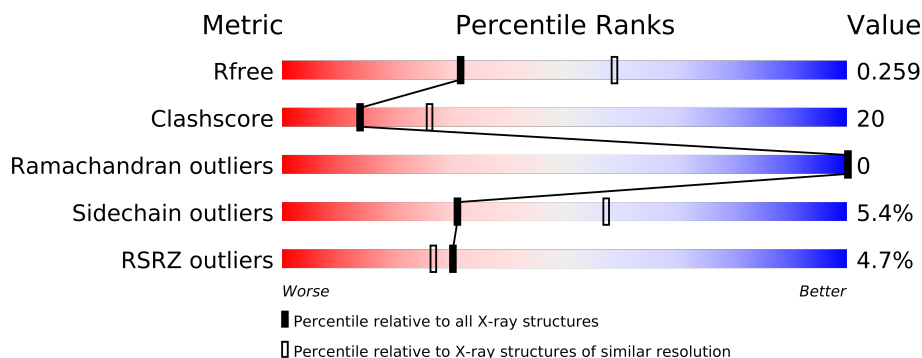
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	107	
1	C	107	
1	E	107	
1	G	107	
2	B	342	
2	D	342	
2	F	342	
2	H	342	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	D	504	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	F	504	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13840 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FK506-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	C	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	E	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			
1	G	107	Total	C	N	O	S	6	0	0
			831	527	146	154	4			

- Molecule 2 is a protein called TGF-B SUPERFAMILY RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			
2	D	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			
2	F	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			
2	H	326	Total	C	N	O	S	17	0	0
			2602	1642	467	477	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	20	Total	O	0	0
			20	20		
4	C	2	Total	O	0	0
			2	2		
4	D	20	Total	O	0	0
			20	20		
4	E	2	Total	O	0	0
			2	2		
4	F	20	Total	O	0	0
			20	20		
4	G	2	Total	O	0	0
			2	2		
4	H	20	Total	O	0	0
			20	20		

### 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 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.

#### • Molecule 1: FK506-BINDING PROTEIN

Chain A:



#### • Molecule 1: FK506-BINDING PROTEIN

Chain C:



#### • Molecule 1: FK506-BINDING PROTEIN

Chain E:



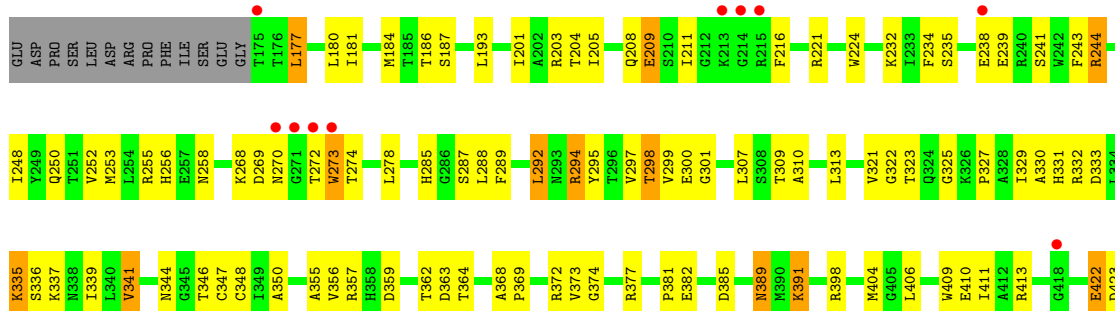
#### • Molecule 1: FK506-BINDING PROTEIN

Chain G:



#### • Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

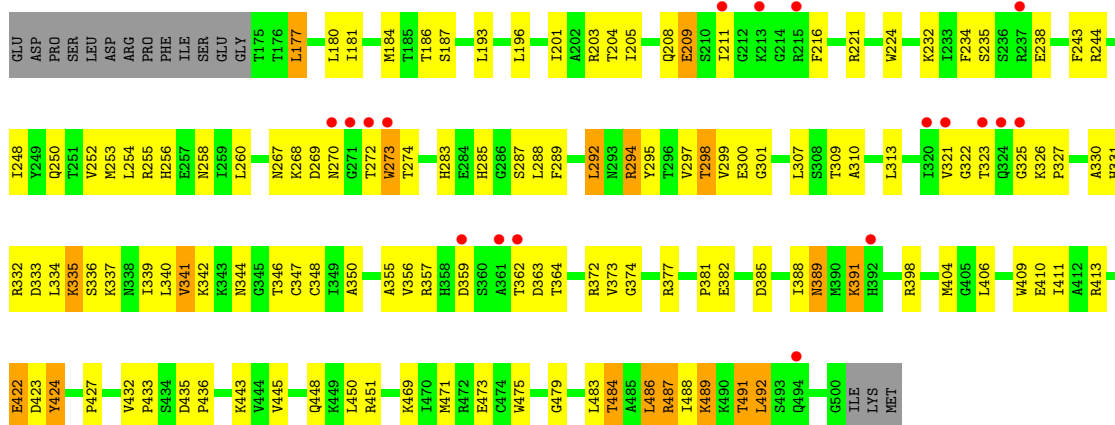
Chain B:





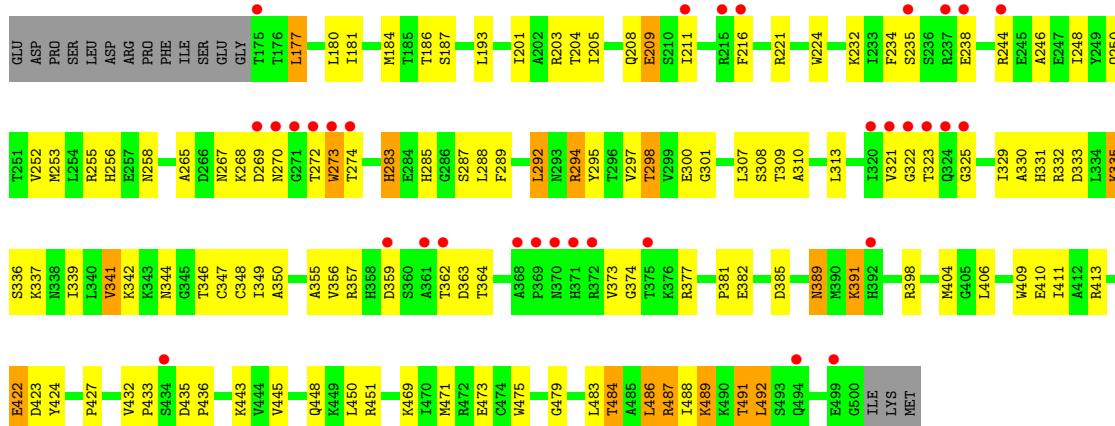
• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain D:



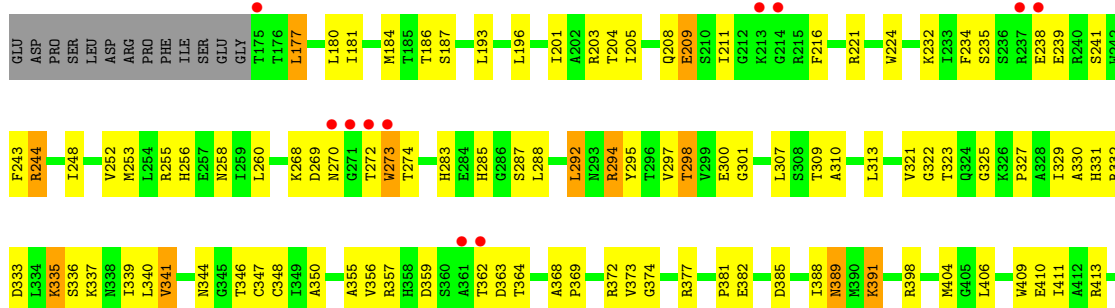
• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain F:



• Molecule 2: TGF-B SUPERFAMILY RECEPTOR TYPE I

Chain H:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.58Å 81.06Å 90.53Å 86.23° 81.86° 63.92°	Depositor
Resolution (Å)	30.00 – 2.60 19.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.60) 90.2 (19.79-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.60 (at 2.59Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, $R_{free}$	0.249 , 0.269 0.238 , 0.259	Depositor DCC
$R_{free}$ test set	5883 reflections (11.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 13.7	EDS
Estimated twinning fraction	0.230 for -h,-h+k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57741 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13840	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/850	0.78	0/1146
1	C	0.48	0/850	0.78	0/1146
1	E	0.48	0/850	0.78	0/1146
1	G	0.48	0/850	0.77	0/1146
2	B	0.61	1/2655 (0.0%)	0.77	1/3586 (0.0%)
2	D	0.61	1/2655 (0.0%)	0.77	1/3586 (0.0%)
2	F	0.62	2/2655 (0.1%)	0.77	2/3586 (0.1%)
2	H	0.62	1/2655 (0.0%)	0.78	2/3586 (0.1%)
All	All	0.59	5/14020 (0.0%)	0.77	6/18928 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	391	LYS	CG-CD	12.69	1.95	1.52
2	D	391	LYS	CG-CD	12.68	1.95	1.52
2	B	391	LYS	CG-CD	12.68	1.95	1.52
2	F	391	LYS	CG-CD	12.65	1.95	1.52
2	F	283	HIS	C-N	-6.20	1.19	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	391	LYS	CB-CG-CD	-7.56	91.94	111.60
2	D	391	LYS	CB-CG-CD	-7.55	91.96	111.60
2	B	391	LYS	CB-CG-CD	-7.55	91.97	111.60
2	F	391	LYS	CB-CG-CD	-7.53	92.01	111.60
2	H	283	HIS	O-C-N	6.61	133.27	122.70
2	F	283	HIS	O-C-N	-5.03	114.65	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	424	TYR	Sidechain
2	D	424	TYR	Sidechain
2	F	424	TYR	Sidechain
2	H	424	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	831	0	831	17	0
1	C	831	0	831	18	0
1	E	831	0	831	24	0
1	G	831	0	831	17	0
2	B	2602	0	2606	125	0
2	D	2602	0	2606	123	0
2	F	2602	0	2605	127	0
2	H	2602	0	2606	120	0
3	B	5	0	0	1	0
3	D	5	0	0	1	0
3	F	5	0	0	1	0
3	H	5	0	0	1	0
4	A	2	0	0	0	0
4	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
4	D	20	0	0	0	0
4	E	2	0	0	0	0
4	F	20	0	0	0	0
4	G	2	0	0	0	0
4	H	20	0	0	0	0
All	All	13840	0	13747	545	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (545) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:484:THR:HG22	2:H:487:ARG:H	1.28	0.97
2:B:484:THR:HG22	2:B:487:ARG:H	1.28	0.97
2:F:484:THR:HG22	2:F:487:ARG:H	1.28	0.94
2:D:484:THR:HG22	2:D:487:ARG:H	1.28	0.94
2:H:216:PHE:CE2	2:H:372:ARG:HD2	2.04	0.92
2:D:216:PHE:CE2	2:D:372:ARG:HD2	2.07	0.89
2:F:443:LYS:HG2	2:F:448:GLN:HE21	1.39	0.87
2:H:443:LYS:HG2	2:H:448:GLN:HE21	1.39	0.87
2:B:443:LYS:HG2	2:B:448:GLN:HE21	1.39	0.86
2:D:443:LYS:HG2	2:D:448:GLN:HE21	1.39	0.85
1:A:66:MET:HA	1:A:70:GLN:OE1	1.78	0.83
2:B:248:ILE:CD1	2:B:355:ALA:HB3	2.11	0.81
2:B:469:LYS:O	2:B:473:GLU:HG2	1.82	0.80
2:B:193:LEU:CD1	2:B:201:ILE:HD12	2.12	0.80
1:E:66:MET:HA	1:E:70:GLN:OE1	1.82	0.80
2:D:209:GLU:OE2	2:D:221:ARG:NH1	2.16	0.79
2:F:469:LYS:O	2:F:473:GLU:HG2	1.82	0.79
2:D:469:LYS:O	2:D:473:GLU:HG2	1.82	0.79
2:F:193:LEU:CD1	2:F:201:ILE:HD12	2.12	0.79
1:A:88:PRO:HG3	2:B:243:PHE:CD1	2.18	0.79
2:F:209:GLU:OE2	2:F:221:ARG:NH1	2.16	0.79
2:B:209:GLU:OE2	2:B:221:ARG:NH1	2.16	0.79
1:C:66:MET:HA	1:C:70:GLN:OE1	1.82	0.79
2:H:209:GLU:OE2	2:H:221:ARG:NH1	2.16	0.79
2:D:193:LEU:CD1	2:D:201:ILE:HD12	2.12	0.79
2:F:252:VAL:HG11	2:F:329:ILE:HD11	1.65	0.79
1:G:66:MET:HA	1:G:70:GLN:OE1	1.82	0.79
2:H:193:LEU:CD1	2:H:201:ILE:HD12	2.12	0.79
2:H:469:LYS:O	2:H:473:GLU:HG2	1.82	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:409:TRP:HD1	2:H:471:MET:HE1	1.48	0.78
2:D:409:TRP:HD1	2:D:471:MET:HE1	1.49	0.77
2:F:409:TRP:HD1	2:F:471:MET:HE1	1.51	0.76
2:B:409:TRP:HD1	2:B:471:MET:HE1	1.51	0.75
2:F:256:HIS:HD2	2:F:258:ASN:H	1.34	0.75
2:H:256:HIS:HD2	2:H:258:ASN:H	1.35	0.74
2:D:310:ALA:HA	2:D:404:MET:HE1	1.69	0.74
2:H:193:LEU:HD13	2:H:201:ILE:HD12	1.69	0.74
2:B:413:ARG:NH1	2:B:423:ASP:O	2.21	0.74
2:F:413:ARG:NH1	2:F:423:ASP:O	2.21	0.73
2:D:409:TRP:CD1	2:D:471:MET:HE1	2.23	0.73
2:B:256:HIS:HD2	2:B:258:ASN:H	1.35	0.73
2:H:413:ARG:NH1	2:H:423:ASP:O	2.21	0.73
2:D:413:ARG:NH1	2:D:423:ASP:O	2.21	0.73
2:D:256:HIS:HD2	2:D:258:ASN:H	1.35	0.73
2:F:310:ALA:HA	2:F:404:MET:HE1	1.71	0.73
2:D:193:LEU:HD13	2:D:201:ILE:HD12	1.69	0.73
2:B:193:LEU:HD13	2:B:201:ILE:HD12	1.69	0.72
2:F:193:LEU:HD13	2:F:201:ILE:HD12	1.69	0.72
2:F:409:TRP:CD1	2:F:471:MET:HE1	2.23	0.72
2:B:409:TRP:CD1	2:B:471:MET:HE1	2.24	0.72
2:H:331:HIS:HD2	2:H:333:ASP:H	1.37	0.72
2:B:252:VAL:HG11	2:B:329:ILE:HD11	1.72	0.72
2:F:298:THR:HG22	2:F:300:GLU:N	2.05	0.71
2:B:298:THR:HG22	2:B:300:GLU:N	2.05	0.71
2:D:331:HIS:HD2	2:D:333:ASP:H	1.37	0.71
2:F:331:HIS:HD2	2:F:333:ASP:H	1.37	0.71
1:A:88:PRO:HG3	2:B:243:PHE:CE1	2.25	0.71
2:D:298:THR:HG22	2:D:300:GLU:N	2.06	0.71
2:H:409:TRP:CD1	2:H:471:MET:HE1	2.25	0.71
2:H:298:THR:HG22	2:H:300:GLU:N	2.06	0.70
2:F:484:THR:CG2	2:F:487:ARG:H	2.04	0.70
2:B:331:HIS:HD2	2:B:333:ASP:H	1.37	0.70
2:D:216:PHE:HD2	2:D:238:GLU:HG2	1.56	0.69
2:B:216:PHE:HD2	2:B:238:GLU:HG2	1.57	0.69
2:B:484:THR:CG2	2:B:487:ARG:H	2.03	0.69
2:F:216:PHE:HD2	2:F:238:GLU:HG2	1.57	0.69
2:D:484:THR:CG2	2:D:487:ARG:H	2.04	0.69
2:H:216:PHE:HD2	2:H:238:GLU:HG2	1.57	0.69
2:B:248:ILE:HD12	2:B:355:ALA:HB3	1.76	0.68
1:G:88:PRO:HG3	2:H:243:PHE:CE1	2.28	0.68
2:F:283:HIS:CE1	2:F:342:LYS:HG2	2.28	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:88:PRO:HG3	2:H:243:PHE:CD1	2.28	0.68
2:F:184:MET:HE3	2:F:193:LEU:HD22	1.75	0.68
2:B:184:MET:HE3	2:B:193:LEU:HD22	1.76	0.67
2:H:310:ALA:HA	2:H:404:MET:CE	2.25	0.67
2:D:184:MET:HE3	2:D:193:LEU:HD22	1.76	0.67
2:H:484:THR:CG2	2:H:487:ARG:H	2.03	0.67
2:D:310:ALA:HA	2:D:404:MET:CE	2.25	0.67
2:D:309:THR:HG22	2:D:404:MET:HE2	1.76	0.67
2:F:309:THR:HG22	2:F:404:MET:HE2	1.77	0.67
2:B:310:ALA:HA	2:B:404:MET:CE	2.25	0.67
2:H:298:THR:HG22	2:H:301:GLY:H	1.60	0.67
2:F:473:GLU:HB3	2:F:483:LEU:HG	1.77	0.66
1:G:42:ARG:HD2	2:H:184:MET:HG2	1.76	0.66
2:F:298:THR:HG22	2:F:301:GLY:H	1.60	0.66
2:F:310:ALA:HA	2:F:404:MET:CE	2.25	0.66
2:B:298:THR:HG22	2:B:301:GLY:H	1.60	0.66
2:F:269:ASP:HA	2:F:274:THR:HA	1.78	0.66
2:H:473:GLU:HB3	2:H:483:LEU:HG	1.78	0.66
2:D:298:THR:HG22	2:D:301:GLY:H	1.61	0.65
2:H:269:ASP:HA	2:H:274:THR:HA	1.78	0.65
2:B:473:GLU:HB3	2:B:483:LEU:HG	1.77	0.65
2:D:269:ASP:HA	2:D:274:THR:HA	1.78	0.65
2:B:269:ASP:HA	2:B:274:THR:HA	1.78	0.64
2:D:473:GLU:HB3	2:D:483:LEU:HG	1.78	0.64
2:H:184:MET:HE3	2:H:193:LEU:HD22	1.78	0.64
1:E:88:PRO:CB	2:F:246:ALA:HB3	2.28	0.63
1:E:90:ILE:CG1	2:F:250:GLN:HG2	2.28	0.63
2:D:216:PHE:CD2	2:D:238:GLU:HG2	2.34	0.62
1:E:90:ILE:HG13	2:F:250:GLN:HG2	1.79	0.62
2:B:310:ALA:HA	2:B:404:MET:HE1	1.82	0.62
2:H:216:PHE:CD2	2:H:238:GLU:HG2	2.35	0.61
2:H:409:TRP:HB2	2:H:471:MET:HE3	1.82	0.61
2:H:310:ALA:HA	2:H:404:MET:HE1	1.81	0.61
2:B:313:LEU:HB3	2:B:404:MET:HE1	1.82	0.61
2:F:211:ILE:HD11	2:F:221:ARG:HB2	1.83	0.61
2:D:331:HIS:CD2	2:D:333:ASP:H	2.18	0.61
2:B:216:PHE:CD2	2:B:238:GLU:HG2	2.35	0.61
2:H:211:ILE:HD11	2:H:221:ARG:HB2	1.83	0.60
2:D:211:ILE:HD11	2:D:221:ARG:HB2	1.83	0.60
2:B:211:ILE:HD11	2:B:221:ARG:HB2	1.83	0.60
2:D:473:GLU:CB	2:D:483:LEU:HG	2.32	0.60
2:F:216:PHE:CD2	2:F:238:GLU:HG2	2.35	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:313:LEU:HB3	2:H:404:MET:HE1	1.82	0.60
2:F:298:THR:HG22	2:F:300:GLU:H	1.67	0.59
2:B:256:HIS:CD2	2:B:258:ASN:H	2.20	0.59
2:H:331:HIS:CD2	2:H:333:ASP:H	2.18	0.59
2:B:298:THR:HG22	2:B:300:GLU:H	1.67	0.59
2:F:331:HIS:CD2	2:F:333:ASP:H	2.18	0.59
2:B:473:GLU:CB	2:B:483:LEU:HG	2.32	0.59
2:F:473:GLU:CB	2:F:483:LEU:HG	2.32	0.59
2:F:204:THR:O	2:F:204:THR:HG22	2.02	0.59
2:H:248:ILE:CD1	2:H:355:ALA:HB3	2.31	0.59
2:H:473:GLU:CB	2:H:483:LEU:HG	2.32	0.59
2:H:260:LEU:HD13	2:H:340:LEU:HD12	1.85	0.59
2:D:336:SER:OG	2:D:410:GLU:OE1	2.21	0.58
2:B:204:THR:HG22	2:B:204:THR:O	2.02	0.58
2:H:377:ARG:HD2	3:H:504:SO4:O2	2.03	0.58
2:D:488:ILE:O	2:D:492:LEU:HB2	2.03	0.58
2:F:256:HIS:CD2	2:F:258:ASN:H	2.19	0.58
2:D:204:THR:HG22	2:D:204:THR:O	2.02	0.58
2:F:377:ARG:HD2	3:F:504:SO4:O2	2.03	0.58
2:D:377:ARG:HD2	3:D:504:SO4:O2	2.03	0.58
2:H:298:THR:HG22	2:H:300:GLU:H	1.68	0.58
2:H:204:THR:O	2:H:204:THR:HG22	2.02	0.58
2:B:336:SER:OG	2:B:410:GLU:OE1	2.21	0.58
2:B:331:HIS:CD2	2:B:333:ASP:H	2.19	0.58
2:H:309:THR:HG22	2:H:404:MET:HE2	1.86	0.58
2:D:298:THR:HG22	2:D:300:GLU:H	1.67	0.57
2:D:232:LYS:HD2	2:D:234:PHE:CZ	2.39	0.57
2:F:488:ILE:O	2:F:492:LEU:HB2	2.04	0.57
2:H:443:LYS:HG2	2:H:448:GLN:NE2	2.17	0.57
2:F:298:THR:CG2	2:F:300:GLU:H	2.18	0.57
1:C:4:VAL:HG22	1:C:74:LEU:HD22	1.87	0.57
2:B:298:THR:CG2	2:B:300:GLU:H	2.17	0.57
2:D:298:THR:CG2	2:D:300:GLU:H	2.18	0.57
2:B:309:THR:HG22	2:B:404:MET:HE2	1.85	0.57
2:H:488:ILE:O	2:H:492:LEU:HB2	2.04	0.57
2:B:377:ARG:HD2	3:B:158:SO4:O2	2.03	0.57
1:E:4:VAL:HG22	1:E:74:LEU:HD22	1.87	0.57
2:F:232:LYS:HD2	2:F:234:PHE:CZ	2.39	0.57
2:B:232:LYS:HD2	2:B:234:PHE:CZ	2.39	0.57
1:G:4:VAL:HG22	1:G:74:LEU:HD22	1.87	0.57
2:B:422:GLU:OE1	2:H:434:SER:HB3	2.05	0.57
2:F:336:SER:OG	2:F:410:GLU:OE1	2.21	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:409:TRP:HB2	2:D:471:MET:HE3	1.87	0.57
2:B:216:PHE:CE2	2:B:372:ARG:HD2	2.40	0.57
2:H:336:SER:OG	2:H:410:GLU:OE1	2.21	0.57
2:H:180:LEU:HG	2:H:184:MET:HE2	1.87	0.57
2:H:232:LYS:HD2	2:H:234:PHE:CZ	2.39	0.56
2:H:256:HIS:CD2	2:H:258:ASN:H	2.20	0.56
2:B:488:ILE:O	2:B:492:LEU:HB2	2.04	0.56
2:B:443:LYS:HG2	2:B:448:GLN:NE2	2.17	0.56
1:G:1:GLY:HA2	1:G:80:TYR:CD1	2.41	0.56
2:F:180:LEU:HG	2:F:184:MET:CE	2.36	0.56
2:D:256:HIS:CD2	2:D:258:ASN:H	2.19	0.56
2:B:252:VAL:HG13	2:B:327:PRO:HD2	1.88	0.56
2:H:298:THR:CG2	2:H:300:GLU:H	2.18	0.56
2:D:248:ILE:CD1	2:D:355:ALA:HB3	2.36	0.56
2:D:288:LEU:HG	2:D:292:LEU:HD22	1.88	0.56
2:H:180:LEU:HG	2:H:184:MET:CE	2.36	0.56
1:A:1:GLY:HA2	1:A:80:TYR:CD1	2.41	0.56
1:C:1:GLY:HA2	1:C:80:TYR:CD1	2.41	0.56
2:B:180:LEU:HG	2:B:184:MET:CE	2.36	0.56
2:F:288:LEU:HG	2:F:292:LEU:HD22	1.88	0.56
2:F:346:THR:CG2	2:F:347:CYS:N	2.70	0.55
2:B:288:LEU:HG	2:B:292:LEU:HD22	1.88	0.55
2:H:288:LEU:HG	2:H:292:LEU:HD22	1.88	0.55
2:D:180:LEU:HG	2:D:184:MET:CE	2.36	0.55
1:E:1:GLY:HA2	1:E:80:TYR:CD1	2.41	0.55
1:A:4:VAL:HG22	1:A:74:LEU:HD22	1.87	0.55
2:F:313:LEU:HB3	2:F:404:MET:HE1	1.89	0.55
2:D:177:LEU:HD13	2:D:224:TRP:CZ3	2.42	0.55
2:F:331:HIS:HE1	2:F:350:ALA:O	1.90	0.55
2:H:346:THR:CG2	2:H:347:CYS:N	2.69	0.55
2:F:443:LYS:HG2	2:F:448:GLN:NE2	2.17	0.54
2:D:346:THR:CG2	2:D:347:CYS:N	2.70	0.54
2:H:177:LEU:HD13	2:H:224:TRP:CZ3	2.42	0.54
2:B:346:THR:CG2	2:B:347:CYS:N	2.70	0.54
2:B:331:HIS:HE1	2:B:350:ALA:O	1.90	0.54
2:B:177:LEU:HD13	2:B:224:TRP:CZ3	2.42	0.54
1:E:88:PRO:HB2	2:F:246:ALA:CB	2.37	0.54
1:E:85:THR:HG21	2:F:267:ASN:HD22	1.73	0.54
2:F:432:VAL:HG13	2:F:433:PRO:HD2	1.90	0.54
2:B:177:LEU:HD11	2:B:201:ILE:HD13	1.90	0.54
2:D:331:HIS:HE1	2:D:350:ALA:O	1.91	0.54
2:D:443:LYS:HG2	2:D:448:GLN:NE2	2.16	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:177:LEU:HD11	2:D:201:ILE:HD13	1.90	0.53
2:D:313:LEU:HB3	2:D:404:MET:HE1	1.90	0.53
2:B:432:VAL:HG13	2:B:433:PRO:HD2	1.90	0.53
2:F:177:LEU:HD13	2:F:224:TRP:CZ3	2.42	0.53
2:H:331:HIS:HE1	2:H:350:ALA:O	1.91	0.53
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.90	0.53
2:H:177:LEU:HD11	2:H:201:ILE:HD13	1.90	0.53
2:B:409:TRP:HB2	2:B:471:MET:HE3	1.91	0.53
2:H:248:ILE:HD12	2:H:355:ALA:HB3	1.91	0.53
2:F:201:ILE:O	2:F:205:ILE:HG13	2.09	0.53
2:D:180:LEU:HG	2:D:184:MET:HE2	1.89	0.53
2:F:177:LEU:HD11	2:F:201:ILE:HD13	1.90	0.52
2:F:258:ASN:C	2:F:348:CYS:HA	2.29	0.52
2:H:432:VAL:HG13	2:H:433:PRO:HD2	1.90	0.52
2:D:433:PRO:O	2:D:436:PRO:HG3	2.10	0.52
2:D:252:VAL:HG13	2:D:327:PRO:HD2	1.91	0.52
2:B:180:LEU:HG	2:B:184:MET:HE2	1.90	0.52
1:E:16:PRO:HG2	1:E:64:ALA:HA	1.92	0.52
2:B:272:THR:HG1	2:B:273:TRP:HE3	1.58	0.52
2:D:258:ASN:O	2:D:348:CYS:HA	2.09	0.52
2:B:288:LEU:HD21	2:B:411:ILE:HD11	1.92	0.52
2:F:433:PRO:O	2:F:436:PRO:HG3	2.09	0.52
2:H:201:ILE:O	2:H:205:ILE:HG13	2.09	0.52
2:F:409:TRP:HB2	2:F:471:MET:HE3	1.92	0.52
2:B:201:ILE:O	2:B:205:ILE:HG13	2.10	0.52
2:D:201:ILE:O	2:D:205:ILE:HG13	2.09	0.52
2:B:433:PRO:O	2:B:436:PRO:HG3	2.10	0.52
1:A:16:PRO:HG2	1:A:64:ALA:HA	1.91	0.52
2:H:216:PHE:CE2	2:H:372:ARG:CD	2.85	0.51
2:F:272:THR:HG1	2:F:273:TRP:HE3	1.57	0.51
1:G:16:PRO:HG2	1:G:64:ALA:HA	1.92	0.51
2:F:180:LEU:HG	2:F:184:MET:HE2	1.92	0.51
1:C:16:PRO:HG2	1:C:64:ALA:HA	1.91	0.51
2:D:193:LEU:HD11	2:D:201:ILE:HD12	1.92	0.51
2:F:288:LEU:HD21	2:F:411:ILE:HD11	1.92	0.51
2:B:244:ARG:NH1	2:B:368:ALA:HB2	2.26	0.51
2:D:253:MET:HE3	2:D:255:ARG:HD2	1.93	0.51
2:H:288:LEU:HD21	2:H:411:ILE:HD11	1.92	0.51
2:B:346:THR:HG22	2:B:347:CYS:N	2.26	0.51
2:D:288:LEU:HD21	2:D:411:ILE:HD11	1.91	0.51
2:F:346:THR:HG22	2:F:347:CYS:N	2.26	0.51
2:H:232:LYS:HD2	2:H:234:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:433:PRO:O	2:H:436:PRO:HG3	2.10	0.50
2:F:248:ILE:CD1	2:F:355:ALA:HB3	2.41	0.50
1:A:42:ARG:HD2	2:B:184:MET:HG2	1.93	0.50
2:D:346:THR:HG22	2:D:347:CYS:N	2.26	0.50
2:H:253:MET:HE3	2:H:255:ARG:HD2	1.93	0.50
2:D:283:HIS:CE1	2:D:342:LYS:HG2	2.46	0.50
2:H:193:LEU:HD11	2:H:201:ILE:HD12	1.92	0.50
2:F:232:LYS:HD2	2:F:234:PHE:CE1	2.46	0.50
2:F:258:ASN:O	2:F:348:CYS:HA	2.12	0.50
2:H:344:ASN:OD1	2:H:346:THR:HB	2.12	0.50
2:D:232:LYS:HD2	2:D:234:PHE:CE1	2.46	0.50
2:F:344:ASN:OD1	2:F:346:THR:HB	2.12	0.50
2:D:248:ILE:HD12	2:D:355:ALA:HB3	1.94	0.50
1:E:88:PRO:HB2	2:F:246:ALA:HB3	1.94	0.49
2:B:232:LYS:HD2	2:B:234:PHE:CE1	2.47	0.49
2:B:344:ASN:OD1	2:B:346:THR:HB	2.12	0.49
2:F:432:VAL:CG1	2:F:436:PRO:HG3	2.43	0.49
2:B:253:MET:HE3	2:B:255:ARG:HD2	1.94	0.49
2:D:272:THR:HG1	2:D:273:TRP:HE3	1.58	0.49
2:D:323:THR:C	2:D:325:GLY:H	2.15	0.49
2:H:272:THR:HG1	2:H:273:TRP:HE3	1.59	0.49
2:D:432:VAL:HG13	2:D:433:PRO:CD	2.43	0.49
2:D:344:ASN:OD1	2:D:346:THR:HB	2.12	0.49
2:F:323:THR:C	2:F:325:GLY:H	2.15	0.49
1:A:50:LEU:HD12	1:A:60:GLU:HG3	1.95	0.49
2:B:432:VAL:CG1	2:B:436:PRO:HG3	2.43	0.49
2:B:323:THR:C	2:B:325:GLY:H	2.15	0.49
1:C:88:PRO:HG3	2:D:243:PHE:CD1	2.48	0.49
2:H:432:VAL:HG13	2:H:433:PRO:CD	2.43	0.48
2:F:471:MET:HE3	2:F:475:TRP:CH2	2.48	0.48
2:H:346:THR:HG22	2:H:347:CYS:N	2.26	0.48
2:D:432:VAL:CG1	2:D:436:PRO:HG3	2.43	0.48
2:B:432:VAL:HG13	2:B:433:PRO:CD	2.43	0.48
2:H:492:LEU:HA	2:H:492:LEU:HD12	1.73	0.48
1:C:50:LEU:HD12	1:C:60:GLU:HG3	1.95	0.48
2:D:258:ASN:C	2:D:348:CYS:HA	2.34	0.48
2:F:432:VAL:HG13	2:F:433:PRO:CD	2.43	0.48
2:H:323:THR:C	2:H:325:GLY:H	2.15	0.48
2:F:362:THR:O	2:F:364:THR:HG23	2.14	0.48
1:E:88:PRO:HB3	2:F:246:ALA:HB3	1.96	0.48
2:B:362:THR:O	2:B:364:THR:HG23	2.14	0.48
2:D:362:THR:O	2:D:364:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:432:VAL:CG1	2:H:436:PRO:HG3	2.43	0.48
1:E:50:LEU:HD12	1:E:60:GLU:HG3	1.95	0.48
1:C:90:ILE:HG13	2:D:250:GLN:HG2	1.94	0.47
2:B:389:ASN:ND2	2:B:391:LYS:H	2.12	0.47
2:F:450:LEU:O	2:F:451:ARG:HD3	2.14	0.47
2:B:471:MET:HE3	2:B:475:TRP:CH2	2.49	0.47
2:B:297:VAL:HG22	2:B:298:THR:N	2.30	0.47
2:F:389:ASN:ND2	2:F:391:LYS:H	2.12	0.47
1:G:50:LEU:HD12	1:G:60:GLU:HG3	1.95	0.47
2:F:253:MET:HE3	2:F:255:ARG:HD2	1.96	0.47
2:D:389:ASN:ND2	2:D:391:LYS:H	2.13	0.47
2:B:193:LEU:HD11	2:B:201:ILE:HD12	1.92	0.47
2:H:297:VAL:HG22	2:H:298:THR:N	2.30	0.47
2:B:450:LEU:O	2:B:451:ARG:HD3	2.15	0.47
2:D:450:LEU:O	2:D:451:ARG:HD3	2.14	0.47
2:H:362:THR:O	2:H:364:THR:HG23	2.14	0.47
2:F:363:ASP:O	2:F:363:ASP:OD1	2.33	0.47
2:F:208:GLN:C	2:F:209:GLU:HG3	2.35	0.47
2:H:208:GLN:C	2:H:209:GLU:HG3	2.35	0.47
2:F:297:VAL:HG22	2:F:298:THR:N	2.30	0.47
2:B:363:ASP:O	2:B:363:ASP:OD1	2.33	0.47
2:F:193:LEU:HD11	2:F:201:ILE:HD12	1.92	0.47
2:D:184:MET:CE	2:D:193:LEU:HD22	2.45	0.47
2:D:270:ASN:C	2:D:272:THR:H	2.18	0.47
1:G:26:TYR:HA	1:G:100:ASP:O	2.15	0.47
2:D:260:LEU:HD13	2:D:340:LEU:HD12	1.97	0.47
2:F:252:VAL:HG11	2:F:329:ILE:CD1	2.42	0.47
2:D:297:VAL:HG22	2:D:298:THR:N	2.30	0.47
2:F:432:VAL:HG12	2:F:433:PRO:O	2.15	0.46
2:B:432:VAL:HG12	2:B:433:PRO:O	2.15	0.46
2:B:484:THR:HG23	2:B:486:LEU:H	1.80	0.46
2:H:450:LEU:O	2:H:451:ARG:HD3	2.15	0.46
2:H:389:ASN:ND2	2:H:391:LYS:H	2.12	0.46
2:D:208:GLN:C	2:D:209:GLU:HG3	2.35	0.46
2:F:492:LEU:HA	2:F:492:LEU:HD12	1.73	0.46
1:C:26:TYR:CZ	2:D:196:LEU:HD22	2.50	0.46
1:A:91:ILE:HA	1:A:92:PRO:HD3	1.83	0.46
2:D:484:THR:HG23	2:D:486:LEU:H	1.80	0.46
2:H:184:MET:CE	2:H:193:LEU:HD22	2.45	0.46
1:G:8:SER:HA	1:G:9:PRO:HD3	1.80	0.46
2:H:432:VAL:HG12	2:H:433:PRO:O	2.16	0.46
2:H:363:ASP:OD1	2:H:363:ASP:O	2.33	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:413:ARG:NH1	2:D:422:GLU:HB3	2.31	0.46
2:D:492:LEU:HD12	2:D:492:LEU:HA	1.73	0.46
1:E:26:TYR:HA	1:E:100:ASP:O	2.15	0.46
1:E:90:ILE:HG12	2:F:250:GLN:HG2	1.97	0.46
2:F:484:THR:HG23	2:F:486:LEU:H	1.80	0.46
2:F:409:TRP:HD1	2:F:471:MET:CE	2.27	0.46
2:B:413:ARG:NH1	2:B:422:GLU:HB3	2.31	0.46
2:H:413:ARG:NH1	2:H:422:GLU:HB3	2.31	0.46
2:D:432:VAL:HG12	2:D:433:PRO:O	2.16	0.46
2:F:270:ASN:C	2:F:272:THR:H	2.18	0.46
2:H:244:ARG:HG2	2:H:368:ALA:CB	2.46	0.46
2:H:373:VAL:HG22	2:H:374:GLY:H	1.81	0.46
2:D:363:ASP:O	2:D:363:ASP:OD1	2.33	0.46
2:B:270:ASN:C	2:B:272:THR:H	2.18	0.45
2:B:357:ARG:HD2	2:B:359:ASP:OD1	2.17	0.45
1:C:26:TYR:HA	1:C:100:ASP:O	2.16	0.45
2:F:258:ASN:ND2	2:F:308:SER:HB2	2.31	0.45
2:H:270:ASN:C	2:H:272:THR:H	2.18	0.45
1:A:26:TYR:HA	1:A:100:ASP:O	2.16	0.45
2:H:484:THR:HG23	2:H:486:LEU:H	1.80	0.45
2:F:413:ARG:NH1	2:F:422:GLU:HB3	2.31	0.45
2:D:410:GLU:OE1	2:D:424:TYR:OH	2.27	0.45
2:H:357:ARG:HD2	2:H:359:ASP:OD1	2.16	0.45
2:B:235:SER:HG	2:B:235:SER:H	1.60	0.45
2:D:471:MET:HE3	2:D:475:TRP:CH2	2.52	0.45
2:D:381:PRO:HD2	2:D:382:GLU:OE2	2.17	0.45
2:H:294:ARG:HD2	2:H:295:TYR:CE1	2.52	0.45
2:D:294:ARG:HD2	2:D:295:TYR:CE1	2.52	0.45
2:D:216:PHE:CZ	2:D:372:ARG:HD2	2.52	0.45
2:H:331:HIS:O	2:H:332:ARG:HB2	2.17	0.45
2:D:331:HIS:O	2:D:332:ARG:HB2	2.17	0.45
2:F:373:VAL:HG22	2:F:374:GLY:H	1.81	0.45
2:B:373:VAL:HG22	2:B:374:GLY:H	1.81	0.45
2:B:381:PRO:HD2	2:B:382:GLU:OE2	2.17	0.45
1:E:90:ILE:HG12	2:F:250:GLN:CG	2.46	0.45
2:F:381:PRO:HD2	2:F:382:GLU:OE2	2.17	0.45
2:D:406:LEU:HB3	2:D:427:PRO:HG2	1.99	0.45
2:B:484:THR:HG22	2:B:487:ARG:N	2.12	0.45
1:A:17:LYS:N	1:A:20:GLN:OE1	2.49	0.45
2:F:294:ARG:HD2	2:F:295:TYR:CE1	2.52	0.45
2:H:381:PRO:HD2	2:H:382:GLU:OE2	2.17	0.45
2:B:294:ARG:HD2	2:B:295:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:85:THR:HG21	2:D:267:ASN:HD22	1.81	0.45
2:F:336:SER:OG	2:F:410:GLU:CD	2.56	0.45
2:F:216:PHE:HD2	2:F:238:GLU:CG	2.28	0.44
2:D:373:VAL:HG22	2:D:374:GLY:H	1.82	0.44
2:D:484:THR:HG22	2:D:487:ARG:N	2.13	0.44
2:D:357:ARG:HD2	2:D:359:ASP:OD1	2.16	0.44
2:H:432:VAL:HG11	2:H:436:PRO:CG	2.48	0.44
2:H:368:ALA:HA	2:H:369:PRO:HD3	1.68	0.44
1:C:17:LYS:N	1:C:20:GLN:OE1	2.49	0.44
2:H:216:PHE:HD2	2:H:238:GLU:CG	2.28	0.44
2:B:336:SER:OG	2:B:410:GLU:CD	2.56	0.44
1:A:1:GLY:HA2	1:A:80:TYR:CG	2.52	0.44
2:D:435:ASP:N	2:D:436:PRO:HD3	2.32	0.44
2:F:406:LEU:HB3	2:F:427:PRO:HG2	2.00	0.44
2:F:184:MET:CE	2:F:193:LEU:HD22	2.46	0.44
2:B:208:GLN:C	2:B:209:GLU:HG3	2.35	0.44
2:F:432:VAL:HG11	2:F:436:PRO:CG	2.47	0.44
2:F:357:ARG:HD2	2:F:359:ASP:OD1	2.17	0.44
1:G:1:GLY:HA2	1:G:80:TYR:CG	2.52	0.44
1:C:1:GLY:HA2	1:C:80:TYR:CG	2.53	0.44
2:B:435:ASP:N	2:B:436:PRO:HD3	2.32	0.44
1:C:84:ALA:O	1:C:93:PRO:CB	2.66	0.44
1:A:84:ALA:O	1:A:93:PRO:CB	2.66	0.44
2:D:177:LEU:O	2:D:181:ILE:HG13	2.18	0.44
2:F:331:HIS:O	2:F:332:ARG:HB2	2.17	0.44
2:B:331:HIS:O	2:B:332:ARG:HB2	2.17	0.44
2:D:203:ARG:NH1	2:D:268:LYS:HG3	2.33	0.44
2:D:177:LEU:HD13	2:D:224:TRP:CE3	2.53	0.44
2:B:409:TRP:HD1	2:B:471:MET:CE	2.27	0.44
2:H:435:ASP:N	2:H:436:PRO:HD3	2.33	0.44
1:E:84:ALA:O	1:E:93:PRO:CB	2.66	0.44
2:B:406:LEU:HB3	2:B:427:PRO:HG2	2.00	0.44
2:H:252:VAL:HG11	2:H:329:ILE:HD11	1.99	0.44
2:H:216:PHE:HE2	2:H:372:ARG:HD2	1.74	0.44
2:B:177:LEU:O	2:B:181:ILE:HG13	2.18	0.44
2:F:177:LEU:O	2:F:181:ILE:HG13	2.18	0.44
2:D:432:VAL:HG11	2:D:436:PRO:CG	2.48	0.44
2:D:335:LYS:HD3	2:D:337:LYS:HB2	2.00	0.44
2:B:278:LEU:HA	2:B:278:LEU:HD12	1.87	0.44
2:D:235:SER:HG	2:D:238:GLU:CD	2.22	0.43
2:B:335:LYS:HD3	2:B:337:LYS:HB2	2.00	0.43
2:B:203:ARG:NH1	2:B:268:LYS:HG3	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:335:LYS:HD3	2:F:337:LYS:HB2	2.00	0.43
1:G:84:ALA:O	1:G:93:PRO:CB	2.66	0.43
2:B:321:VAL:HG12	2:B:322:GLY:N	2.33	0.43
2:H:406:LEU:HB3	2:H:427:PRO:HG2	2.00	0.43
2:B:216:PHE:HD2	2:B:238:GLU:CG	2.28	0.43
2:D:321:VAL:HG12	2:D:322:GLY:N	2.33	0.43
2:F:203:ARG:NH1	2:F:268:LYS:HG3	2.33	0.43
1:E:1:GLY:HA2	1:E:80:TYR:CG	2.53	0.43
2:H:177:LEU:HD13	2:H:224:TRP:CE3	2.53	0.43
2:B:186:THR:O	2:B:187:SER:C	2.57	0.43
2:F:484:THR:HG22	2:F:487:ARG:N	2.13	0.43
2:B:177:LEU:HD13	2:B:224:TRP:CE3	2.53	0.43
2:H:331:HIS:HD2	2:H:333:ASP:N	2.12	0.43
2:F:235:SER:HG	2:F:238:GLU:CD	2.21	0.43
2:B:432:VAL:HG11	2:B:436:PRO:CG	2.48	0.43
2:F:385:ASP:C	2:F:385:ASP:OD1	2.57	0.43
2:D:186:THR:O	2:D:187:SER:C	2.57	0.43
2:F:177:LEU:HD13	2:F:224:TRP:CE3	2.53	0.43
2:F:389:ASN:C	2:F:389:ASN:HD22	2.22	0.43
2:B:398:ARG:HD3	2:B:479:GLY:C	2.39	0.43
2:H:385:ASP:OD1	2:H:385:ASP:C	2.57	0.43
2:D:398:ARG:HD3	2:D:479:GLY:C	2.39	0.43
2:H:177:LEU:O	2:H:181:ILE:HG13	2.18	0.43
2:D:336:SER:OG	2:D:410:GLU:CD	2.56	0.43
2:F:435:ASP:N	2:F:436:PRO:HD3	2.32	0.43
1:C:8:SER:HA	1:C:9:PRO:HD3	1.81	0.43
1:E:87:HIS:HE1	2:F:265:ALA:O	2.02	0.43
2:B:391:LYS:O	2:B:391:LYS:HG2	2.19	0.43
2:H:203:ARG:NH1	2:H:268:LYS:HG3	2.33	0.43
2:F:432:VAL:CG1	2:F:436:PRO:CG	2.97	0.43
2:D:391:LYS:O	2:D:391:LYS:HG2	2.19	0.43
1:E:17:LYS:N	1:E:20:GLN:OE1	2.49	0.43
2:H:336:SER:OG	2:H:410:GLU:CD	2.57	0.42
2:H:389:ASN:C	2:H:389:ASN:HD22	2.23	0.42
2:H:391:LYS:O	2:H:391:LYS:HG2	2.19	0.42
1:E:91:ILE:HA	1:E:92:PRO:HD3	1.83	0.42
2:B:487:ARG:O	2:B:491:THR:HG23	2.19	0.42
2:B:252:VAL:HG11	2:B:329:ILE:CD1	2.46	0.42
2:H:335:LYS:HD3	2:H:337:LYS:HB2	2.00	0.42
2:H:321:VAL:HG12	2:H:322:GLY:N	2.33	0.42
2:B:368:ALA:HA	2:B:369:PRO:HD3	1.68	0.42
2:H:330:ALA:HB3	2:H:356:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:180:LEU:HG	2:F:184:MET:HE1	2.01	0.42
2:F:391:LYS:HG2	2:F:391:LYS:O	2.19	0.42
1:C:91:ILE:HA	1:C:92:PRO:HD3	1.83	0.42
2:F:398:ARG:HD3	2:F:479:GLY:C	2.39	0.42
2:D:385:ASP:OD1	2:D:385:ASP:C	2.57	0.42
2:B:184:MET:CE	2:B:193:LEU:HD22	2.45	0.42
1:E:90:ILE:HD11	2:F:250:GLN:OE1	2.20	0.42
2:D:432:VAL:CG1	2:D:436:PRO:CG	2.97	0.42
2:B:244:ARG:HG2	2:B:368:ALA:CB	2.49	0.42
2:H:398:ARG:HD3	2:H:479:GLY:C	2.39	0.42
2:B:389:ASN:HD22	2:B:389:ASN:C	2.22	0.42
2:B:330:ALA:HB3	2:B:356:VAL:HG22	2.02	0.42
2:D:331:HIS:HD2	2:D:333:ASP:N	2.12	0.42
2:F:321:VAL:HG12	2:F:322:GLY:N	2.33	0.42
2:H:235:SER:H	2:H:235:SER:HG	1.60	0.42
2:B:385:ASP:OD1	2:B:385:ASP:C	2.57	0.42
2:F:330:ALA:HB3	2:F:356:VAL:HG22	2.02	0.42
2:H:487:ARG:O	2:H:491:THR:HG23	2.20	0.42
2:D:216:PHE:HD2	2:D:238:GLU:CG	2.28	0.42
1:E:88:PRO:HB2	2:F:246:ALA:HB1	2.02	0.42
2:D:389:ASN:C	2:D:389:ASN:HD22	2.22	0.42
1:G:105:LYS:HE3	1:G:107:GLU:OE2	2.20	0.42
1:C:71:ARG:HA	1:C:101:VAL:O	2.20	0.42
2:F:186:THR:O	2:F:187:SER:C	2.57	0.42
2:D:487:ARG:O	2:D:491:THR:HG23	2.19	0.42
2:H:238:GLU:O	2:H:239:GLU:C	2.58	0.42
2:B:177:LEU:HD12	2:B:177:LEU:HA	1.87	0.42
2:H:432:VAL:CG1	2:H:436:PRO:CG	2.97	0.42
2:D:330:ALA:HB3	2:D:356:VAL:HG22	2.01	0.42
1:A:105:LYS:HE3	1:A:107:GLU:OE2	2.20	0.42
1:G:71:ARG:HA	1:G:101:VAL:O	2.20	0.42
2:H:489:LYS:HD2	2:H:489:LYS:C	2.41	0.42
2:F:177:LEU:HD12	2:F:177:LEU:HA	1.87	0.42
2:B:432:VAL:CG1	2:B:436:PRO:CG	2.97	0.42
1:A:90:ILE:HG13	2:B:250:GLN:HG2	2.02	0.42
2:H:186:THR:O	2:H:187:SER:C	2.57	0.41
2:F:489:LYS:C	2:F:489:LYS:HD2	2.41	0.41
1:A:71:ARG:HA	1:A:101:VAL:O	2.20	0.41
2:F:487:ARG:O	2:F:491:THR:HG23	2.19	0.41
2:B:248:ILE:HD13	2:B:355:ALA:HB3	1.97	0.41
2:H:471:MET:HE3	2:H:475:TRP:CH2	2.55	0.41
2:B:238:GLU:O	2:B:239:GLU:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:252:VAL:HG13	2:H:327:PRO:HD2	2.02	0.41
2:D:186:THR:HG22	2:D:187:SER:N	2.36	0.41
2:B:285:HIS:HB2	2:B:341:VAL:O	2.20	0.41
2:D:445:VAL:HG13	2:D:451:ARG:NH1	2.36	0.41
2:B:489:LYS:HD2	2:B:489:LYS:C	2.41	0.41
2:D:285:HIS:HB2	2:D:341:VAL:O	2.20	0.41
2:F:204:THR:O	2:F:204:THR:CG2	2.69	0.41
2:B:270:ASN:C	2:B:272:THR:N	2.74	0.41
1:G:26:TYR:CZ	2:H:196:LEU:HD22	2.56	0.41
2:F:180:LEU:HD12	2:F:180:LEU:HA	1.96	0.41
2:B:410:GLU:OE1	2:B:424:TYR:OH	2.26	0.41
2:H:285:HIS:HB2	2:H:341:VAL:O	2.21	0.41
2:D:254:LEU:HD21	2:D:326:LYS:HE2	2.02	0.41
2:D:334:LEU:HD23	2:D:334:LEU:HA	1.90	0.41
1:C:105:LYS:HE3	1:C:107:GLU:OE2	2.20	0.41
2:B:186:THR:HG22	2:B:187:SER:N	2.35	0.41
2:D:287:SER:HA	2:D:339:ILE:O	2.21	0.41
2:F:216:PHE:HB3	2:F:238:GLU:HG2	2.03	0.41
1:C:90:ILE:CG1	2:D:250:GLN:HG2	2.50	0.41
2:F:331:HIS:HD2	2:F:333:ASP:N	2.12	0.41
2:B:216:PHE:HB3	2:B:238:GLU:HG2	2.03	0.41
2:F:270:ASN:C	2:F:272:THR:N	2.74	0.41
2:H:270:ASN:C	2:H:272:THR:N	2.74	0.41
2:B:445:VAL:HG13	2:B:451:ARG:NH1	2.35	0.41
2:H:445:VAL:HG13	2:H:451:ARG:NH1	2.35	0.41
1:E:71:ARG:HA	1:E:101:VAL:O	2.20	0.41
2:H:388:ILE:O	2:H:388:ILE:HG23	2.21	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41
2:F:289:PHE:HB2	2:F:336:SER:HB2	2.03	0.41
2:D:270:ASN:C	2:D:272:THR:N	2.74	0.41
2:F:287:SER:HA	2:F:339:ILE:O	2.21	0.41
2:B:287:SER:HA	2:B:339:ILE:O	2.21	0.41
2:D:298:THR:CG2	2:D:299:VAL:N	2.84	0.40
2:B:238:GLU:HB3	2:B:241:SER:HB2	2.03	0.40
2:B:289:PHE:HB2	2:B:336:SER:HB2	2.03	0.40
2:D:272:THR:OG1	2:D:273:TRP:HE3	2.04	0.40
1:E:105:LYS:HE3	1:E:107:GLU:OE2	2.20	0.40
1:G:91:ILE:HA	1:G:92:PRO:HD3	1.83	0.40
2:B:272:THR:OG1	2:B:273:TRP:HE3	2.04	0.40
2:F:445:VAL:HG13	2:F:451:ARG:NH1	2.36	0.40
2:F:285:HIS:HB2	2:F:341:VAL:O	2.20	0.40
1:G:17:LYS:N	1:G:20:GLN:OE1	2.49	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:258:ASN:O	2:B:348:CYS:HA	2.21	0.40
2:B:298:THR:CG2	2:B:299:VAL:N	2.84	0.40
2:D:289:PHE:HB2	2:D:336:SER:HB2	2.03	0.40
2:H:272:THR:OG1	2:H:273:TRP:HE3	2.04	0.40
2:H:186:THR:HG22	2:H:187:SER:N	2.36	0.40
2:D:388:ILE:O	2:D:388:ILE:HG23	2.21	0.40
2:D:489:LYS:C	2:D:489:LYS:HD2	2.41	0.40
2:H:238:GLU:HB3	2:H:241:SER:HB2	2.03	0.40
2:D:184:MET:HE3	2:D:193:LEU:CD2	2.50	0.40
2:F:258:ASN:O	2:F:349:ILE:N	2.45	0.40
2:H:258:ASN:O	2:H:348:CYS:HA	2.22	0.40
2:H:287:SER:HA	2:H:339:ILE:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	C	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
1	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	B	324/342 (95%)	306 (94%)	18 (6%)	0	100	100
2	D	324/342 (95%)	307 (95%)	17 (5%)	0	100	100
2	F	324/342 (95%)	306 (94%)	18 (6%)	0	100	100
2	H	324/342 (95%)	307 (95%)	17 (5%)	0	100	100
All	All	1716/1796 (96%)	1622 (94%)	94 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	89/89 (100%)	87 (98%)	2 (2%)	64	89
1	C	89/89 (100%)	87 (98%)	2 (2%)	64	89
1	E	89/89 (100%)	87 (98%)	2 (2%)	64	89
1	G	89/89 (100%)	87 (98%)	2 (2%)	64	89
2	B	279/294 (95%)	261 (94%)	18 (6%)	24	46
2	D	279/294 (95%)	261 (94%)	18 (6%)	24	46
2	F	279/294 (95%)	261 (94%)	18 (6%)	24	46
2	H	279/294 (95%)	261 (94%)	18 (6%)	24	46
All	All	1472/1532 (96%)	1392 (95%)	80 (5%)	31	57

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	59	TRP
2	B	177	LEU
2	B	209	GLU
2	B	244	ARG
2	B	273	TRP
2	B	292	LEU
2	B	294	ARG
2	B	298	THR
2	B	307	LEU
2	B	335	LYS
2	B	341	VAL
2	B	389	ASN
2	B	422	GLU
2	B	484	THR
2	B	486	LEU
2	B	487	ARG
2	B	489	LYS
2	B	491	THR
2	B	492	LEU
1	C	25	HIS

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Mol	Chain	Res	Type
1	C	59	TRP
2	D	177	LEU
2	D	209	GLU
2	D	244	ARG
2	D	273	TRP
2	D	292	LEU
2	D	294	ARG
2	D	298	THR
2	D	307	LEU
2	D	335	LYS
2	D	341	VAL
2	D	389	ASN
2	D	422	GLU
2	D	484	THR
2	D	486	LEU
2	D	487	ARG
2	D	489	LYS
2	D	491	THR
2	D	492	LEU
1	E	25	HIS
1	E	59	TRP
2	F	177	LEU
2	F	209	GLU
2	F	244	ARG
2	F	273	TRP
2	F	292	LEU
2	F	294	ARG
2	F	298	THR
2	F	307	LEU
2	F	335	LYS
2	F	341	VAL
2	F	389	ASN
2	F	422	GLU
2	F	484	THR
2	F	486	LEU
2	F	487	ARG
2	F	489	LYS
2	F	491	THR
2	F	492	LEU
1	G	25	HIS
1	G	59	TRP
2	H	177	LEU

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Mol	Chain	Res	Type
2	H	209	GLU
2	H	244	ARG
2	H	273	TRP
2	H	292	LEU
2	H	294	ARG
2	H	298	THR
2	H	307	LEU
2	H	335	LYS
2	H	341	VAL
2	H	389	ASN
2	H	422	GLU
2	H	484	THR
2	H	486	LEU
2	H	487	ARG
2	H	489	LYS
2	H	491	THR
2	H	492	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	256	HIS
2	B	315	HIS
2	B	331	HIS
2	B	389	ASN
2	B	448	GLN
2	B	494	GLN
1	C	87	HIS
2	D	256	HIS
2	D	258	ASN
2	D	331	HIS
2	D	389	ASN
2	D	448	GLN
2	D	494	GLN
1	E	87	HIS
2	F	256	HIS
2	F	267	ASN
2	F	315	HIS
2	F	331	HIS
2	F	389	ASN
2	F	448	GLN
2	F	494	GLN

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Mol	Chain	Res	Type
2	H	256	HIS
2	H	331	HIS
2	H	389	ASN
2	H	448	GLN
2	H	494	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

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	B	158	-	4,4,4	0.59	0	6,6,6	0.13	0
3	SO4	D	504	-	4,4,4	0.64	0	6,6,6	0.14	0
3	SO4	F	504	-	4,4,4	0.66	0	6,6,6	0.13	0
3	SO4	H	504	-	4,4,4	0.61	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	158	-	-	0/0/0/0	0/0/0/0
3	SO4	D	504	-	-	0/0/0/0	0/0/0/0
3	SO4	F	504	-	-	0/0/0/0	0/0/0/0
3	SO4	H	504	-	-	0/0/0/0	0/0/0/0

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.

## 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 ⓘ

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	107/107 (100%)	0.09	0	100	100	31, 40, 51, 57	2 (1%)
1	C	107/107 (100%)	0.16	3 (2%)	50	48	31, 40, 52, 58	2 (1%)
1	E	107/107 (100%)	0.24	2 (1%)	64	61	32, 41, 52, 58	2 (1%)
1	G	107/107 (100%)	0.15	1 (0%)	81	82	31, 40, 51, 57	2 (1%)
2	B	326/342 (95%)	0.15	11 (3%)	43	39	13, 31, 66, 85	5 (1%)
2	D	326/342 (95%)	0.28	18 (5%)	24	20	15, 32, 66, 86	5 (1%)
2	F	326/342 (95%)	0.57	33 (10%)	7	5	16, 33, 66, 86	5 (1%)
2	H	326/342 (95%)	0.18	12 (3%)	39	35	15, 31, 66, 86	5 (1%)
All	All	1732/1796 (96%)	0.26	80 (4%)	30	27	13, 36, 60, 86	28 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	270	ASN	8.2
2	D	272	THR	7.6
2	D	324	GLN	7.5
2	H	271	GLY	7.4
2	F	271	GLY	7.0
2	F	371	HIS	6.8
2	F	324	GLN	6.8
2	F	272	THR	6.3
2	F	322	GLY	6.2
2	H	272	THR	6.1
2	F	269	ASP	6.0
2	B	272	THR	6.0
2	F	321	VAL	5.8
2	F	273	TRP	5.7
2	F	369	PRO	5.7
2	B	271	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
2	F	323	THR	5.2
2	F	237	ARG	4.9
2	D	325	GLY	4.9
2	D	273	TRP	4.8
2	F	361	ALA	4.8
2	D	271	GLY	4.8
2	F	216	PHE	4.6
2	D	323	THR	4.5
2	D	494	GLN	4.4
2	D	270	ASN	4.2
2	F	368	ALA	4.2
2	F	372	ARG	4.2
2	B	214	GLY	4.0
2	D	320	ILE	3.9
2	H	213	LYS	3.9
2	B	273	TRP	3.8
2	F	370	ASN	3.7
2	B	215	ARG	3.7
2	F	235	SER	3.5
2	F	325	GLY	3.5
2	F	320	ILE	3.4
2	B	270	ASN	3.4
2	F	238	GLU	3.4
2	D	321	VAL	3.3
2	H	270	ASN	3.2
2	H	273	TRP	3.1
2	D	359	ASP	3.1
2	F	359	ASP	3.1
2	D	237	ARG	3.0
2	D	215	ARG	3.0
2	F	215	ARG	2.9
2	F	494	GLN	2.9
2	F	244	ARG	2.8
2	B	499	GLU	2.8
2	D	362	THR	2.8
2	D	361	ALA	2.7
2	F	434	SER	2.6
2	D	211	ILE	2.5
2	F	499	GLU	2.5
2	B	418	GLY	2.5
2	F	362	THR	2.5
2	H	362	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	238	GLU	2.4
2	F	375	THR	2.4
2	B	213	LYS	2.4
2	H	237	ARG	2.3
2	H	499	GLU	2.3
1	C	32	ASP	2.3
2	H	175	THR	2.3
1	C	18	ARG	2.3
1	E	1	GLY	2.2
2	D	213	LYS	2.2
2	F	392	HIS	2.2
2	H	361	ALA	2.2
1	E	34	LYS	2.2
2	B	175	THR	2.1
2	F	274	THR	2.1
1	C	34	LYS	2.1
2	F	211	ILE	2.1
2	H	214	GLY	2.0
2	D	392	HIS	2.0
2	B	238	GLU	2.0
1	G	18	ARG	2.0
2	F	175	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	504	5/5	0.35	8.46	63,64,64,65	0
3	SO4	F	504	5/5	0.56	4.43	64,64,65,66	0
3	SO4	B	158	5/5	0.16	-0.46	61,61,62,62	0
3	SO4	H	504	5/5	0.15	-1.34	62,62,62,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.