



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:31 AM GMT

PDB ID : 2XD1  
Title : ACTIVE SITE RESTRUCTURING REGULATES LIGAND RECOGNITION IN CLASS A PENICILLIN-BINDING PROTEINS  
Authors : Macheboeuf, P.; Di Guilmi, A.M.; Job, V.; Vernet, T.; Dideberg, O.; Dessen, A.  
Deposited on : 2010-04-28  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

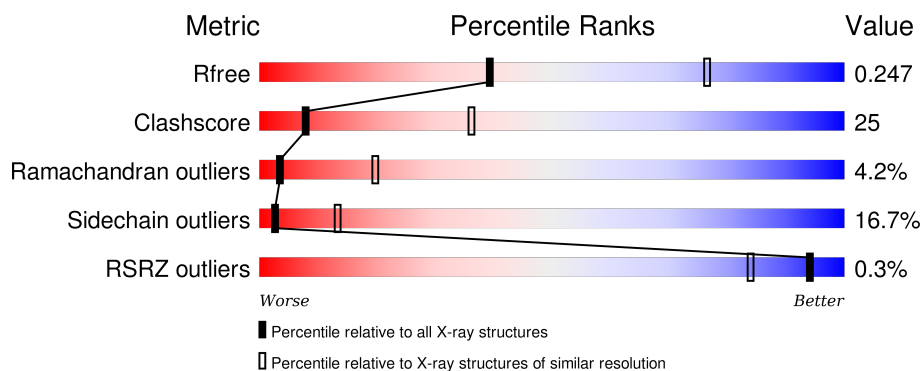
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 46%, orange 37%, yellow 11%, green 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>46%</span> <span>37%</span> <span>11%</span> <span>• 5%</span> </div> </div>
1	B	494	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 45%, orange 34%, yellow 11%, green 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>45%</span> <span>34%</span> <span>11%</span> <span>• 8%</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7278 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.

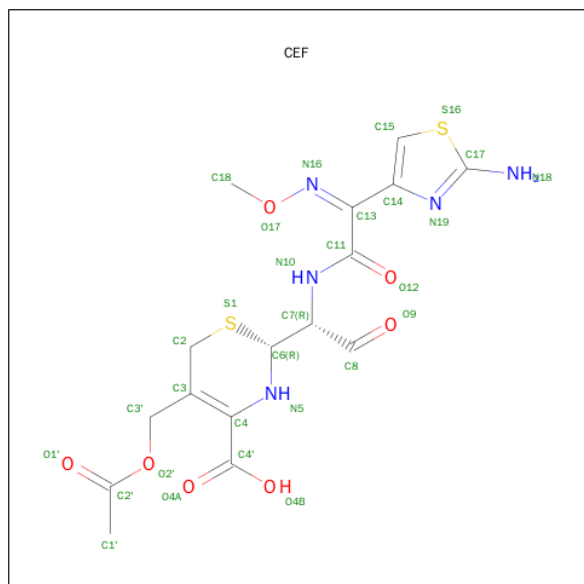
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3617	2263	613	726	15			
1	B	455	Total	C	N	O	S	0	0	0
			3508	2195	594	704	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
A	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	686	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4
B	687	GLN	ARG	ENGINEERED MUTATION	UNP Q7CRA4

- Molecule 2 is CEFOTAXIME GROUP (three-letter code: CEF) (formula:  $C_{16}H_{19}N_5O_7S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		
2	B	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is SULFATE ION (three-letter code: 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		

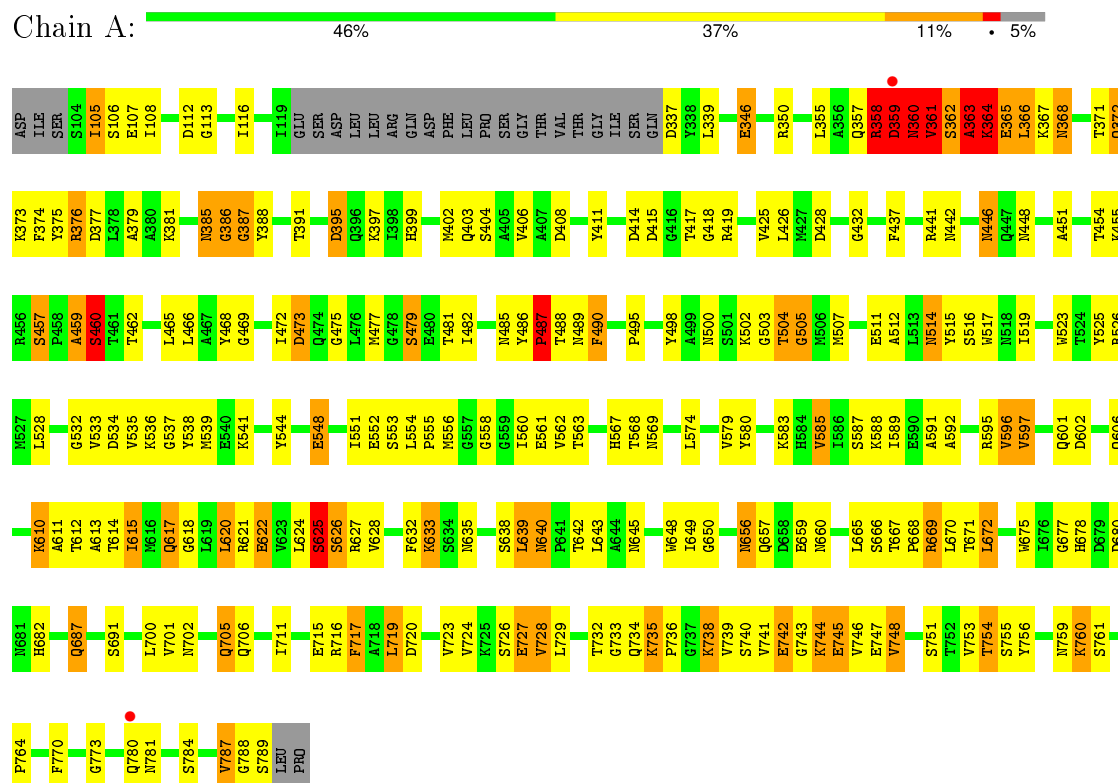
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	47	Total	O	0	0
			47	47		

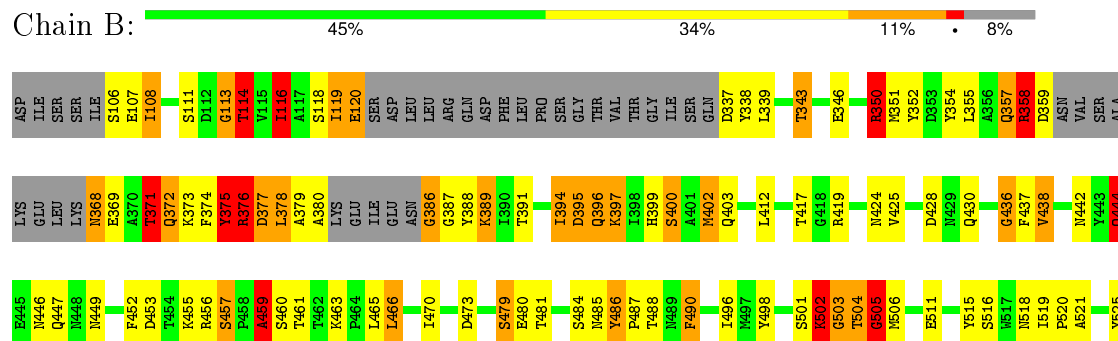
### 3 Residue-property plots

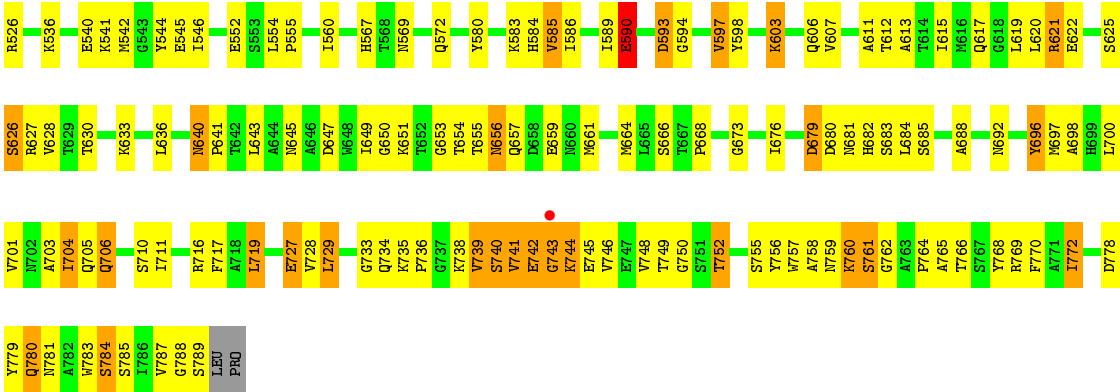
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PENICILLIN-BINDING PROTEIN 1B



#### • Molecule 1: PENICILLIN-BINDING PROTEIN 1B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.60Å 102.30Å 146.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 3.00 45.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.22-3.00) 99.7 (45.20-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.74 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.161 , 0.248 0.163 , 0.247	Depositor DCC
$R_{free}$ test set	2955 reflections (11.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29671 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7278	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 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CEF, 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	1.62	38/3690 (1.0%)	1.48	36/5009 (0.7%)
1	B	1.64	45/3579 (1.3%)	1.44	34/4858 (0.7%)
All	All	1.63	83/7269 (1.1%)	1.46	70/9867 (0.7%)

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
1	A	0	2
1	B	0	4
All	All	0	6

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	LYS	C-N	16.50	1.62	1.33
1	A	459	ALA	C-N	15.84	1.70	1.34
1	A	727	GLU	CG-CD	10.67	1.68	1.51
1	A	460	SER	C-N	9.04	1.54	1.34
1	A	346	GLU	CG-CD	8.79	1.65	1.51
1	B	727	GLU	CG-CD	8.18	1.64	1.51
1	A	486	TYR	CE1-CZ	8.02	1.49	1.38
1	B	503	GLY	C-O	7.88	1.36	1.23
1	B	505	GLY	N-CA	7.77	1.57	1.46
1	B	503	GLY	CA-C	7.67	1.64	1.51
1	B	346	GLU	CG-CD	7.63	1.63	1.51
1	B	346	GLU	CB-CG	7.62	1.66	1.52
1	B	505	GLY	C-N	7.53	1.51	1.34
1	A	346	GLU	CB-CG	7.38	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	484	SER	CB-OG	7.19	1.51	1.42
1	A	346	GLU	CD-OE2	6.97	1.33	1.25
1	B	107	GLU	CD-OE1	6.89	1.33	1.25
1	A	425	VAL	CB-CG1	6.86	1.67	1.52
1	B	375	TYR	CD2-CE2	6.78	1.49	1.39
1	A	748	VAL	CB-CG2	6.73	1.67	1.52
1	B	505	GLY	C-O	6.44	1.33	1.23
1	A	363	ALA	N-CA	6.41	1.59	1.46
1	A	361	VAL	CB-CG2	-6.30	1.39	1.52
1	A	511	GLU	CG-CD	6.30	1.61	1.51
1	B	425	VAL	CB-CG2	-6.30	1.39	1.52
1	B	490	PHE	CG-CD2	6.25	1.48	1.38
1	A	388	TYR	CB-CG	-6.25	1.42	1.51
1	B	120	GLU	CG-CD	6.18	1.61	1.51
1	B	606	GLN	CG-CD	6.17	1.65	1.51
1	B	515	TYR	CE1-CZ	6.14	1.46	1.38
1	A	374	PHE	CE2-CZ	6.05	1.48	1.37
1	A	451	ALA	CA-CB	-6.04	1.39	1.52
1	B	400	SER	CB-OG	-6.03	1.34	1.42
1	A	633	LYS	CD-CE	6.01	1.66	1.51
1	B	379	ALA	CA-CB	5.96	1.65	1.52
1	A	360	ASN	CB-CG	5.93	1.64	1.51
1	A	548	GLU	CB-CG	5.87	1.63	1.52
1	A	580	TYR	CG-CD2	5.83	1.46	1.39
1	B	444	GLN	CG-CD	5.81	1.64	1.51
1	A	701	VAL	CB-CG1	-5.79	1.40	1.52
1	B	107	GLU	CD-OE2	5.75	1.31	1.25
1	B	419	ARG	C-O	5.75	1.34	1.23
1	B	375	TYR	CE2-CZ	5.68	1.46	1.38
1	A	648	TRP	CZ3-CH2	-5.64	1.31	1.40
1	B	498	TYR	CE1-CZ	5.59	1.45	1.38
1	B	585	VAL	CB-CG2	-5.57	1.41	1.52
1	A	432	GLY	N-CA	5.56	1.54	1.46
1	B	375	TYR	CG-CD1	5.56	1.46	1.39
1	B	703	ALA	CA-CB	-5.55	1.40	1.52
1	A	511	GLU	CD-OE1	5.51	1.31	1.25
1	B	626	SER	C-O	-5.50	1.12	1.23
1	A	716	ARG	CG-CD	5.49	1.65	1.51
1	A	105	ILE	CA-CB	5.49	1.67	1.54
1	B	696	TYR	CE2-CZ	-5.48	1.31	1.38
1	B	358	ARG	CG-CD	5.47	1.65	1.51
1	B	698	ALA	CA-CB	-5.46	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TYR	CG-CD1	5.46	1.46	1.39
1	B	506	MET	CA-CB	-5.41	1.42	1.53
1	B	438	VAL	CA-CB	-5.41	1.43	1.54
1	B	727	GLU	CD-OE2	5.38	1.31	1.25
1	A	568	THR	CA-CB	-5.37	1.39	1.53
1	A	595	ARG	CG-CD	5.36	1.65	1.51
1	B	757	TRP	CG-CD1	5.35	1.44	1.36
1	B	502	LYS	N-CA	5.34	1.57	1.46
1	B	375	TYR	CD1-CE1	5.30	1.47	1.39
1	A	727	GLU	CB-CG	5.30	1.62	1.52
1	B	727	GLU	CD-OE1	5.29	1.31	1.25
1	A	359	ASP	CB-CG	5.25	1.62	1.51
1	B	490	PHE	CE1-CZ	5.25	1.47	1.37
1	B	486	TYR	C-O	5.24	1.33	1.23
1	A	490	PHE	CE1-CZ	5.23	1.47	1.37
1	A	360	ASN	CA-C	5.20	1.66	1.52
1	B	586	ILE	CA-CB	5.16	1.66	1.54
1	B	114	THR	CA-CB	5.16	1.66	1.53
1	B	116	ILE	CA-CB	5.15	1.66	1.54
1	B	511	GLU	CD-OE2	5.13	1.31	1.25
1	A	515	TYR	CZ-OH	-5.13	1.29	1.37
1	A	406	VAL	CB-CG2	-5.08	1.42	1.52
1	A	363	ALA	CA-CB	5.08	1.63	1.52
1	A	512	ALA	CA-CB	-5.06	1.41	1.52
1	B	486	TYR	CD2-CE2	-5.06	1.31	1.39
1	A	648	TRP	CE3-CZ3	5.05	1.47	1.38
1	A	415	ASP	CB-CG	5.03	1.62	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	SER	O-C-N	-13.25	101.50	122.70
1	A	428	ASP	CB-CG-OD1	9.71	127.04	118.30
1	B	395	ASP	CB-CG-OD2	9.40	126.76	118.30
1	A	395	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	A	459	ALA	O-C-N	-9.39	107.68	122.70
1	A	395	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	459	ALA	CA-C-N	-8.22	99.11	117.20
1	B	526	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	A	669	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	536	LYS	CD-CE-NZ	-7.78	93.81	111.70
1	B	546	ILE	C-N-CD	7.75	144.68	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	394	ILE	CG1-CB-CG2	-7.23	95.50	111.40
1	A	376	ARG	NE-CZ-NH2	7.23	123.91	120.30
1	A	460	SER	C-N-CA	-7.21	103.69	121.70
1	A	408	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	360	ASN	CB-CA-C	6.92	124.23	110.40
1	B	729	LEU	CA-CB-CG	6.83	131.02	115.30
1	B	114	THR	N-CA-CB	6.80	123.23	110.30
1	A	373	LYS	CD-CE-NZ	-6.79	96.09	111.70
1	B	395	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	A	574	LEU	CB-CG-CD1	-6.63	99.73	111.00
1	B	762	GLY	N-CA-C	-6.62	96.54	113.10
1	A	717	PHE	N-CA-C	-6.46	93.56	111.00
1	B	113	GLY	N-CA-C	-6.46	96.96	113.10
1	A	735	LYS	CD-CE-NZ	-6.38	97.03	111.70
1	B	679	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	556	MET	CG-SD-CE	-6.35	90.04	100.20
1	A	414	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	504	THR	C-N-CA	-6.30	109.08	122.30
1	B	590	GLU	N-CA-CB	6.27	121.88	110.60
1	B	419	ARG	CG-CD-NE	-6.18	98.81	111.80
1	A	337	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	358	ARG	N-CA-C	-6.06	94.64	111.00
1	B	350	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	B	375	TYR	CA-CB-CG	-6.04	101.92	113.40
1	B	554	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	B	526	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	506	MET	CB-CA-C	-5.88	98.65	110.40
1	B	502	LYS	CD-CE-NZ	-5.87	98.20	111.70
1	B	436	GLY	N-CA-C	-5.87	98.43	113.10
1	A	428	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	455	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	B	526	ARG	CG-CD-NE	5.80	123.97	111.80
1	A	473	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	620	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	A	500	ASN	N-CA-C	5.56	126.02	111.00
1	A	534	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	456	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	639	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	672	LEU	CA-CB-CG	-5.52	102.59	115.30
1	A	388	TYR	CB-CA-C	-5.48	99.45	110.40
1	A	358	ARG	CG-CD-NE	5.44	123.23	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	LYS	CD-CE-NZ	-5.43	99.20	111.70
1	A	627	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	358	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	402	MET	CG-SD-CE	5.32	108.70	100.20
1	A	667	THR	C-N-CD	5.31	139.54	128.40
1	B	505	GLY	N-CA-C	5.30	126.35	113.10
1	B	636	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	A	625	SER	CA-CB-OG	-5.29	96.93	111.20
1	B	386	GLY	N-CA-C	5.27	126.27	113.10
1	B	750	GLY	N-CA-C	-5.24	100.00	113.10
1	A	751	SER	N-CA-CB	5.22	118.34	110.50
1	B	444	GLN	N-CA-CB	-5.20	101.24	110.60
1	B	378	LEU	CB-CG-CD1	5.16	119.76	111.00
1	A	669	ARG	CB-CG-CD	-5.12	98.27	111.60
1	B	466	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	362	SER	N-CA-C	5.06	124.67	111.00
1	B	704	ILE	CG1-CB-CG2	-5.01	100.39	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ASP	Peptide
1	A	460	SER	Mainchain
1	B	371	THR	Peptide
1	B	375	TYR	Peptide
1	B	459	ALA	Mainchain
1	B	666	SER	Peptide

## 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	3617	0	3484	161	1
1	B	3508	0	3363	189	0
2	A	26	0	12	2	0
2	B	26	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	44	0	0	3	0
4	B	47	0	0	6	0
All	All	7278	0	6871	350	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 25.

All (350) 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:116:ILE:CD1	1:B:116:ILE:CG1	1.82	1.53
1:A:459:ALA:C	1:A:460:SER:N	1.70	1.41
1:B:376:ARG:NH1	1:B:380:ALA:HB2	1.47	1.28
1:B:373:LYS:O	1:B:376:ARG:HB3	1.49	1.10
1:B:706:GLN:NE2	1:B:706:GLN:HA	1.69	1.05
1:B:376:ARG:HH12	1:B:380:ALA:HB2	0.90	1.02
1:B:734:GLN:HG2	1:B:764:PRO:HG2	1.40	1.02
1:A:687:GLN:OE1	1:A:687:GLN:HA	1.59	0.98
1:B:706:GLN:HE21	1:B:706:GLN:CA	1.78	0.96
1:B:376:ARG:NH1	1:B:380:ALA:CB	2.29	0.94
1:A:643:LEU:HD22	1:A:705:GLN:CG	1.98	0.94
1:A:643:LEU:HD22	1:A:705:GLN:HG2	1.50	0.93
1:A:376:ARG:HD3	4:A:2005:HOH:O	1.68	0.93
1:A:720:ASP:O	1:A:723:VAL:HG23	1.68	0.92
1:B:108:ILE:HD13	1:B:343:THR:CG2	2.00	0.92
1:B:459:ALA:HB1	2:B:1460:CEF:O9	1.70	0.90
1:B:706:GLN:HE21	1:B:706:GLN:HA	1.33	0.88
1:B:621:ARG:HD2	4:B:2027:HOH:O	1.73	0.86
1:B:525:TYR:HB2	1:B:555:PRO:HG3	1.56	0.86
1:A:642:THR:O	1:A:645:ASN:HB2	1.77	0.85
1:B:108:ILE:HD13	1:B:343:THR:HG22	1.60	0.83
1:B:376:ARG:HG3	1:B:377:ASP:N	1.94	0.83
1:A:402:MET:HG2	1:A:700:LEU:HD11	1.61	0.83
1:A:732:THR:O	1:A:734:GLN:N	2.12	0.82
1:B:680:ASP:OD1	1:B:682:HIS:HD2	1.61	0.82
1:A:481:THR:HG22	1:A:482:ILE:H	1.45	0.81
1:B:417:THR:O	1:B:682:HIS:HE1	1.62	0.81
1:A:687:GLN:CA	1:A:687:GLN:OE1	2.29	0.81
1:A:358:ARG:HH11	1:A:358:ARG:HG2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:CD1	1:B:343:THR:CG2	2.62	0.78
1:B:108:ILE:HG23	1:B:116:ILE:HG23	1.65	0.77
1:A:640:ASN:HD22	1:A:640:ASN:C	1.88	0.77
1:A:358:ARG:O	1:A:360:ASN:N	2.16	0.77
1:A:362:SER:HB2	1:A:366:LEU:HD22	1.67	0.77
1:A:622:GLU:O	1:A:626:SER:HB3	1.85	0.76
1:A:741:VAL:O	1:A:742:GLU:HG2	1.86	0.76
1:B:376:ARG:HH12	1:B:380:ALA:CB	1.85	0.74
1:B:743:GLY:O	1:B:744:LYS:HB2	1.86	0.74
1:B:358:ARG:HH11	1:B:358:ARG:CG	2.00	0.73
1:B:729:LEU:HD21	1:B:736:PRO:HB3	1.71	0.73
1:A:668:PRO:HA	1:A:717:PHE:CZ	2.24	0.72
1:A:680:ASP:OD1	1:A:682:HIS:HD2	1.73	0.72
1:A:715:GLU:H	1:A:715:GLU:CD	1.93	0.72
1:B:697:MET:O	1:B:701:VAL:HG23	1.89	0.72
1:A:728:VAL:HG12	1:A:735:LYS:N	2.05	0.71
1:B:645:ASN:O	1:B:716:ARG:NH2	2.24	0.71
1:B:741:VAL:HG12	1:B:741:VAL:O	1.91	0.71
1:B:778:ASP:OD2	4:B:2047:HOH:O	2.07	0.71
1:B:485:ASN:HD22	1:B:520:PRO:HD3	1.56	0.70
1:B:118:SER:C	1:B:119:ILE:HD13	2.11	0.70
1:A:537:GLY:O	1:A:541:LYS:HG3	1.92	0.69
1:B:377:ASP:C	1:B:377:ASP:OD2	2.31	0.69
1:A:362:SER:HB2	1:A:366:LEU:CD2	2.22	0.69
1:B:358:ARG:HH11	1:B:358:ARG:HG2	1.57	0.69
1:B:544:TYR:OH	1:B:567:HIS:HD2	1.74	0.69
1:B:399:HIS:HD2	1:B:436:GLY:HA2	1.57	0.69
1:B:376:ARG:CG	1:B:377:ASP:N	2.56	0.68
1:B:337:ASP:HA	4:B:2004:HOH:O	1.92	0.68
1:A:745:GLU:HG3	1:A:745:GLU:O	1.94	0.68
1:B:354:TYR:CZ	1:B:597:VAL:HG12	2.29	0.68
1:A:363:ALA:O	1:A:365:GLU:N	2.27	0.67
1:B:743:GLY:O	1:B:744:LYS:CB	2.41	0.67
1:A:739:VAL:HG12	1:A:740:SER:H	1.60	0.67
1:B:375:TYR:CD1	1:B:375:TYR:N	2.61	0.67
1:B:633:LYS:NZ	4:B:2031:HOH:O	2.27	0.66
1:A:739:VAL:HG12	1:A:740:SER:N	2.09	0.66
1:A:385:ASN:O	1:A:387:GLY:N	2.28	0.66
1:A:426:LEU:HD11	1:A:670:LEU:HD13	1.77	0.66
1:B:780:GLN:CG	1:B:781:ASN:N	2.59	0.66
1:B:403:GLN:NE2	1:B:403:GLN:HA	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:GLN:HE21	1:B:706:GLN:N	1.94	0.64
1:B:611:ALA:O	1:B:615:ILE:HG13	1.98	0.64
1:A:643:LEU:HD22	1:A:705:GLN:HG3	1.77	0.64
1:A:621:ARG:HB2	1:A:649:ILE:HG22	1.78	0.64
1:B:481:THR:HG23	4:B:2044:HOH:O	1.97	0.64
1:A:362:SER:CB	1:A:366:LEU:HD22	2.28	0.63
1:B:358:ARG:HB3	1:B:358:ARG:NH1	2.13	0.63
1:B:542:MET:HA	1:B:580:TYR:CE1	2.34	0.63
1:B:380:ALA:O	1:B:386:GLY:CA	2.47	0.63
1:A:544:TYR:OH	1:A:567:HIS:HD2	1.80	0.63
1:A:640:ASN:C	1:A:640:ASN:ND2	2.52	0.63
1:B:465:LEU:O	1:B:470:ILE:HG13	1.98	0.63
1:B:380:ALA:O	1:B:386:GLY:N	2.31	0.63
1:A:729:LEU:HD21	1:A:736:PRO:HB3	1.81	0.63
1:A:417:THR:OG1	1:A:678:HIS:HE1	1.82	0.62
1:B:424:ASN:HB2	1:B:438:VAL:HB	1.82	0.62
1:B:358:ARG:O	1:B:359:ASP:C	2.38	0.62
1:A:760:LYS:H	1:A:760:LYS:HD3	1.63	0.62
1:A:734:GLN:HG2	1:A:764:PRO:HG2	1.82	0.61
1:B:613:ALA:O	1:B:617:GLN:HG3	2.00	0.61
1:B:569:ASN:O	1:B:572:GLN:HB3	2.01	0.61
1:B:116:ILE:O	1:B:116:ILE:HD12	2.01	0.61
1:A:368:ASN:HD21	1:A:371:THR:H	1.48	0.61
1:A:669:ARG:HD3	4:A:2039:HOH:O	1.99	0.60
1:B:503:GLY:C	1:B:504:THR:HG23	2.21	0.60
1:A:606:GLN:HE22	1:A:610:LYS:HG2	1.67	0.60
1:B:654:THR:HG23	1:B:661:MET:CE	2.32	0.60
1:B:680:ASP:OD1	1:B:682:HIS:CD2	2.51	0.60
1:A:485:ASN:HD22	1:A:519:ILE:HB	1.66	0.60
1:B:627:ARG:HG3	1:B:627:ARG:HH11	1.67	0.59
1:B:358:ARG:NH1	1:B:359:ASP:OD1	2.30	0.59
1:B:108:ILE:CD1	1:B:343:THR:HG22	2.31	0.59
1:B:741:VAL:CG1	1:B:741:VAL:O	2.51	0.59
1:A:368:ASN:ND2	1:A:371:THR:H	1.99	0.59
1:B:368:ASN:O	1:B:368:ASN:ND2	2.22	0.59
1:B:739:VAL:HG23	1:B:748:VAL:HG23	1.85	0.59
1:B:461:THR:OG1	1:B:567:HIS:HE1	1.86	0.59
1:B:503:GLY:O	1:B:504:THR:CG2	2.50	0.59
1:A:479:SER:HB3	1:A:756:TYR:HB2	1.85	0.58
1:B:680:ASP:O	1:B:681:ASN:HB2	2.04	0.58
1:B:351:MET:O	1:B:354:TYR:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:MET:HG2	1:B:700:LEU:HD11	1.86	0.58
1:B:760:LYS:HG2	1:B:761:SER:N	2.19	0.58
1:B:490:PHE:CZ	1:B:496:ILE:HG12	2.38	0.57
1:B:640:ASN:HD22	1:B:640:ASN:C	2.08	0.57
1:B:640:ASN:ND2	1:B:643:LEU:H	2.02	0.57
1:A:738:LYS:HD2	1:A:747:GLU:OE2	2.04	0.57
1:B:457:SER:HB2	1:B:560:ILE:O	2.04	0.57
1:A:614:THR:HA	1:A:617:GLN:HG3	1.87	0.57
1:A:552:GLU:HG3	4:A:2024:HOH:O	2.04	0.57
1:A:728:VAL:HG12	1:A:734:GLN:C	2.24	0.57
1:A:596:VAL:HG12	1:A:596:VAL:O	2.05	0.57
1:B:473:ASP:HA	1:B:612:THR:OG1	2.05	0.57
1:B:350:ARG:HD2	1:B:598:TYR:CE2	2.40	0.56
1:B:626:SER:HB2	1:B:628:VAL:HG23	1.87	0.56
1:A:360:ASN:O	1:A:362:SER:N	2.39	0.56
1:B:119:ILE:HD13	1:B:119:ILE:N	2.20	0.56
1:B:368:ASN:O	1:B:369:GLU:OE1	2.23	0.56
1:A:411:TYR:HA	1:A:441:ARG:NH2	2.21	0.56
1:B:108:ILE:CG2	1:B:116:ILE:HG23	2.33	0.55
1:A:632:PHE:HA	1:A:635:ASN:HD22	1.69	0.55
1:B:501:SER:C	1:B:503:GLY:H	2.09	0.55
1:B:536:LYS:O	1:B:540:GLU:HB2	2.07	0.55
1:A:360:ASN:O	1:A:361:VAL:C	2.45	0.55
1:B:485:ASN:HD22	1:B:519:ILE:HB	1.71	0.55
1:B:541:LYS:HB2	1:B:607:VAL:HG22	1.89	0.55
1:B:485:ASN:ND2	1:B:520:PRO:HD3	2.22	0.55
1:A:481:THR:HG22	1:A:482:ILE:N	2.20	0.55
1:B:358:ARG:HH11	1:B:358:ARG:CB	2.20	0.55
1:A:760:LYS:HG2	1:A:761:SER:N	2.22	0.55
1:B:503:GLY:O	1:B:504:THR:HG23	2.07	0.54
1:A:362:SER:O	1:A:363:ALA:O	2.24	0.54
1:B:525:TYR:CB	1:B:555:PRO:HG3	2.32	0.54
1:B:378:LEU:HB3	1:B:388:TYR:CE2	2.43	0.54
1:B:396:GLN:O	1:B:396:GLN:HG3	2.06	0.54
1:B:656:ASN:O	1:B:657:GLN:HB2	2.08	0.54
1:A:459:ALA:HB1	2:A:1460:CEF:O9	2.08	0.54
1:B:544:TYR:OH	1:B:567:HIS:CD2	2.59	0.54
1:B:355:LEU:HD22	1:B:358:ARG:NH2	2.23	0.53
1:B:621:ARG:NH2	1:B:647:ASP:OD2	2.40	0.53
1:B:350:ARG:HD2	1:B:598:TYR:CZ	2.42	0.53
1:A:780:GLN:O	1:A:784:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:TYR:HB2	1:A:555:PRO:HG3	1.90	0.53
1:A:544:TYR:OH	1:A:567:HIS:CD2	2.61	0.53
1:B:668:PRO:HD3	1:B:717:PHE:CE2	2.43	0.53
1:B:621:ARG:HH21	1:B:647:ASP:CG	2.13	0.53
1:B:108:ILE:CD1	1:B:343:THR:HG23	2.39	0.52
1:A:399:HIS:O	1:A:403:GLN:HG2	2.08	0.52
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.72	0.52
1:A:419:ARG:O	1:A:678:HIS:CD2	2.62	0.52
1:A:675:TRP:CZ2	1:A:677:GLY:HA3	2.44	0.52
1:B:688:ALA:HA	1:B:692:ASN:HB2	1.92	0.52
1:B:417:THR:HG21	1:B:683:SER:O	2.10	0.52
1:A:468:TYR:O	1:A:469:GLY:C	2.48	0.52
1:B:734:GLN:NE2	1:B:770:PHE:HB2	2.24	0.52
1:B:399:HIS:CD2	1:B:436:GLY:HA2	2.42	0.52
1:B:479:SER:HG	1:B:756:TYR:H	1.57	0.52
1:A:639:LEU:O	1:A:640:ASN:HB2	2.10	0.52
1:B:371:THR:HB	1:B:374:PHE:CD2	2.45	0.52
1:A:489:ASN:OD1	1:A:495:PRO:HA	2.08	0.52
1:B:108:ILE:HG21	1:B:343:THR:HG21	1.92	0.52
1:A:459:ALA:CB	1:A:460:SER:N	2.73	0.51
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.74	0.51
1:A:665:LEU:O	1:A:671:THR:HG23	2.10	0.51
1:A:446:ASN:OD1	1:A:446:ASN:C	2.48	0.51
1:A:504:THR:O	1:A:505:GLY:C	2.48	0.51
1:A:472:ILE:HA	1:A:477:MET:O	2.10	0.51
1:B:106:SER:HB2	1:B:387:GLY:H	1.74	0.51
1:B:728:VAL:O	1:B:752:THR:HG22	2.11	0.51
1:B:680:ASP:CG	1:B:682:HIS:HD2	2.14	0.51
1:A:360:ASN:O	1:A:362:SER:OG	2.25	0.51
1:B:650:GLY:HA2	1:B:664:MET:O	2.11	0.51
1:A:375:TYR:O	1:A:376:ARG:C	2.44	0.51
1:B:611:ALA:HB3	1:B:758:ALA:HB1	1.93	0.51
1:A:734:GLN:NE2	1:A:770:PHE:HB3	2.26	0.50
1:A:610:LYS:HE2	1:A:720:ASP:OD1	2.11	0.50
1:A:743:GLY:O	1:A:744:LYS:C	2.49	0.50
1:A:624:LEU:HD11	1:A:649:ILE:C	2.32	0.50
1:B:643:LEU:HD22	1:B:705:GLN:HG3	1.93	0.50
1:B:424:ASN:ND2	1:B:696:TYR:OH	2.44	0.50
1:A:362:SER:O	1:A:365:GLU:OE2	2.29	0.50
1:A:620:LEU:HD22	1:A:650:GLY:O	2.12	0.50
1:A:460:SER:N	2:A:1460:CEF:O9	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:O	1:A:379:ALA:HB3	2.12	0.50
1:A:760:LYS:H	1:A:760:LYS:CD	2.24	0.50
1:B:375:TYR:HD1	1:B:375:TYR:N	2.09	0.50
1:B:759:ASN:HB2	1:B:760:LYS:HD3	1.93	0.50
1:B:389:LYS:HB3	1:B:590:GLU:OE2	2.11	0.50
1:B:339:LEU:O	1:B:343:THR:HB	2.12	0.50
1:A:346:GLU:OE1	1:A:585:VAL:HB	2.12	0.50
1:A:551:ILE:HG22	1:A:553:SER:H	1.77	0.50
1:A:643:LEU:CD2	1:A:705:GLN:HG2	2.33	0.49
1:A:358:ARG:NH1	1:A:360:ASN:OD1	2.45	0.49
1:A:746:VAL:HG12	1:A:747:GLU:O	2.11	0.49
1:A:732:THR:C	1:A:734:GLN:H	2.16	0.49
1:B:622:GLU:HB3	4:B:2028:HOH:O	2.11	0.49
1:B:446:ASN:OD1	1:B:446:ASN:C	2.50	0.49
1:B:376:ARG:HG3	1:B:377:ASP:H	1.71	0.49
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.24	0.49
1:A:787:VAL:O	1:A:789:SER:N	2.46	0.49
1:B:449:ASN:O	1:B:453:ASP:HB2	2.11	0.49
1:A:702:ASN:O	1:A:705:GLN:HB3	2.12	0.49
1:A:742:GLU:CG	1:A:742:GLU:O	2.60	0.49
1:A:399:HIS:CD2	1:A:437:PHE:H	2.31	0.49
1:B:654:THR:HG23	1:B:661:MET:SD	2.52	0.49
1:A:487:PRO:O	1:A:488:THR:HB	2.12	0.49
1:A:371:THR:O	1:A:372:GLN:C	2.51	0.48
1:A:656:ASN:O	1:A:659:GLU:HG3	2.13	0.48
1:A:485:ASN:HB3	1:A:507:MET:HE3	1.94	0.48
1:A:726:SER:O	1:A:754:THR:HA	2.13	0.48
1:A:418:GLY:O	1:A:419:ARG:C	2.51	0.48
1:B:113:GLY:O	1:B:114:THR:CB	2.61	0.48
1:A:457:SER:HB2	1:A:560:ILE:O	2.13	0.48
1:A:459:ALA:O	1:A:460:SER:N	2.39	0.48
1:B:485:ASN:HB3	1:B:505:GLY:O	2.13	0.48
1:B:760:LYS:HG2	1:B:761:SER:H	1.78	0.48
1:A:620:LEU:HD23	1:A:620:LEU:HA	1.57	0.48
1:B:768:TYR:CE2	1:B:783:TRP:CD1	3.01	0.48
1:B:734:GLN:HB2	1:B:766:THR:HA	1.96	0.48
1:B:486:TYR:CE1	1:B:505:GLY:HA2	2.48	0.48
1:B:734:GLN:HE22	1:B:770:PHE:CB	2.27	0.48
1:A:622:GLU:HA	1:A:625:SER:HB2	1.96	0.47
1:B:357:GLN:C	1:B:357:GLN:CD	2.71	0.47
1:A:485:ASN:HB3	1:A:507:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:CD	1:A:715:GLU:N	2.64	0.47
1:A:487:PRO:HG3	1:A:502:LYS:O	2.15	0.47
1:B:784:SER:OG	1:B:785:SER:N	2.47	0.47
1:A:528:LEU:HD22	1:A:533:VAL:HG21	1.96	0.47
1:B:403:GLN:HA	1:B:403:GLN:HE21	1.80	0.47
1:A:760:LYS:HG2	1:A:761:SER:H	1.79	0.47
1:A:523:TRP:CG	1:A:773:GLY:HA3	2.49	0.47
1:B:378:LEU:O	1:B:386:GLY:HA2	2.14	0.47
1:B:417:THR:O	1:B:682:HIS:CE1	2.54	0.47
1:B:357:GLN:C	1:B:358:ARG:O	2.53	0.47
1:A:112:ASP:OD1	1:A:113:GLY:N	2.48	0.47
1:B:460:SER:HB2	1:B:653:GLY:HA2	1.97	0.47
1:A:358:ARG:HH12	1:A:360:ASN:HD21	1.62	0.47
1:B:640:ASN:HA	1:B:641:PRO:HD3	1.59	0.47
1:B:376:ARG:HG3	1:B:377:ASP:HB3	1.97	0.46
1:A:462:THR:HB	1:A:555:PRO:O	2.16	0.46
1:B:783:TRP:O	1:B:784:SER:C	2.53	0.46
1:A:569:ASN:HD21	1:A:583:LYS:H	1.62	0.46
1:B:108:ILE:O	1:B:116:ILE:N	2.43	0.46
1:A:473:ASP:HA	1:A:612:THR:OG1	2.15	0.46
1:B:473:ASP:HB2	1:B:612:THR:HG21	1.96	0.46
1:A:441:ARG:O	1:A:442:ASN:HB2	2.15	0.46
1:A:466:LEU:O	1:A:466:LEU:HD23	2.16	0.46
1:A:738:LYS:HA	1:A:746:VAL:O	2.15	0.46
1:B:729:LEU:CD2	1:B:736:PRO:HB3	2.42	0.46
1:A:739:VAL:CG1	1:A:740:SER:N	2.78	0.46
1:B:729:LEU:CD1	1:B:748:VAL:HG12	2.45	0.46
1:B:729:LEU:HD13	1:B:748:VAL:HG12	1.96	0.46
1:B:738:LYS:HA	1:B:746:VAL:O	2.15	0.46
1:A:579:VAL:O	1:A:579:VAL:HG12	2.14	0.46
1:B:452:PHE:N	1:B:452:PHE:CD2	2.84	0.46
1:B:625:SER:O	1:B:627:ARG:HG3	2.16	0.46
1:A:514:ASN:O	1:A:628:VAL:HB	2.16	0.46
1:B:740:SER:O	1:B:742:GLU:N	2.49	0.45
1:A:357:GLN:O	1:A:359:ASP:N	2.49	0.45
1:B:688:ALA:O	1:B:692:ASN:HB2	2.16	0.45
1:B:460:SER:HA	1:B:463:LYS:HE3	1.98	0.45
1:B:375:TYR:O	1:B:377:ASP:N	2.50	0.45
1:B:780:GLN:HG3	1:B:781:ASN:N	2.20	0.45
1:B:760:LYS:H	1:B:760:LYS:CD	2.30	0.45
1:B:735:LYS:HB2	1:B:765:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LEU:HD12	1:A:558:GLY:O	2.17	0.45
1:A:350:ARG:NH1	1:A:350:ARG:HG2	2.32	0.45
1:B:487:PRO:O	1:B:488:THR:HB	2.17	0.45
1:A:455:LYS:HA	1:A:562:VAL:O	2.17	0.45
1:A:615:ILE:HD11	1:A:723:VAL:HG13	1.99	0.45
1:B:661:MET:HB2	1:B:676:ILE:HG12	1.99	0.45
1:A:498:TYR:CD1	1:A:517:TRP:HA	2.52	0.45
1:A:615:ILE:HD13	1:A:756:TYR:CB	2.47	0.45
1:A:569:ASN:ND2	1:A:583:LYS:H	2.15	0.45
1:A:611:ALA:O	1:A:615:ILE:HG13	2.17	0.44
1:A:739:VAL:CG1	1:A:740:SER:H	2.26	0.44
1:B:542:MET:HG3	1:B:607:VAL:HG21	1.99	0.44
1:B:116:ILE:HG12	1:B:339:LEU:HG	1.99	0.44
1:A:640:ASN:HD21	1:A:643:LEU:H	1.64	0.44
1:A:734:GLN:NE2	1:A:770:PHE:CB	2.80	0.44
1:B:504:THR:O	1:B:505:GLY:O	2.36	0.44
1:A:618:GLY:HA2	1:A:621:ARG:NH1	2.32	0.44
1:A:402:MET:HG2	1:A:700:LEU:CD1	2.41	0.44
1:B:485:ASN:ND2	1:B:519:ILE:HB	2.33	0.44
1:A:671:THR:HG22	1:A:672:LEU:N	2.33	0.44
1:A:612:THR:HG22	1:A:613:ALA:N	2.32	0.43
1:A:596:VAL:CG1	1:A:596:VAL:O	2.66	0.43
1:A:723:VAL:HG12	1:A:724:VAL:N	2.34	0.43
1:B:706:GLN:NE2	1:B:706:GLN:CA	2.39	0.43
1:A:503:GLY:C	1:A:504:THR:HG23	2.39	0.43
1:A:589:ILE:HB	1:A:597:VAL:HG12	1.99	0.43
1:B:620:LEU:HD23	1:B:620:LEU:HA	1.84	0.43
1:A:539:MET:O	1:A:544:TYR:HB2	2.18	0.43
1:B:734:GLN:NE2	1:B:770:PHE:CB	2.82	0.43
1:B:521:ALA:O	1:B:555:PRO:HG2	2.19	0.43
1:A:459:ALA:CA	1:A:460:SER:N	2.73	0.43
1:A:728:VAL:HG21	1:A:755:SER:HB2	2.00	0.43
1:A:671:THR:CG2	1:A:672:LEU:N	2.82	0.43
1:A:454:THR:O	1:A:563:THR:HG22	2.19	0.42
1:B:375:TYR:C	1:B:377:ASP:H	2.23	0.42
1:B:503:GLY:C	1:B:504:THR:CG2	2.86	0.42
1:A:485:ASN:ND2	1:A:519:ILE:HB	2.34	0.42
1:A:391:THR:HG22	1:A:587:SER:OG	2.19	0.42
1:B:372:GLN:HE21	1:B:372:GLN:HB3	1.65	0.42
1:B:446:ASN:OD1	1:B:447:GLN:N	2.53	0.42
1:B:352:TYR:C	1:B:352:TYR:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:MET:HA	1:B:580:TYR:CD1	2.54	0.42
1:A:613:ALA:O	1:A:617:GLN:HG2	2.19	0.42
1:B:424:ASN:HA	1:B:673:GLY:O	2.20	0.42
1:A:643:LEU:C	1:A:645:ASN:N	2.70	0.42
1:A:362:SER:HA	1:A:365:GLU:OE2	2.19	0.42
1:A:364:LYS:HD3	1:A:364:LYS:C	2.40	0.42
1:A:614:THR:HA	1:A:617:GLN:CG	2.48	0.42
1:B:772:ILE:H	1:B:772:ILE:HG12	1.45	0.42
1:A:668:PRO:HA	1:A:717:PHE:CE1	2.54	0.42
1:B:655:THR:O	1:B:656:ASN:C	2.59	0.42
1:B:685:SER:H	1:B:685:SER:HG	1.59	0.41
1:B:375:TYR:C	1:B:377:ASP:N	2.74	0.41
1:B:437:PHE:C	1:B:437:PHE:CD1	2.93	0.41
1:A:385:ASN:HB2	1:A:386:GLY:H	1.76	0.41
1:B:376:ARG:HD2	1:B:376:ARG:C	2.41	0.41
1:B:487:PRO:HG3	1:B:502:LYS:O	2.21	0.41
1:B:787:VAL:O	1:B:789:SER:N	2.53	0.41
1:B:480:GLU:HB2	1:B:755:SER:HB2	2.03	0.41
1:B:622:GLU:HA	1:B:625:SER:HB2	2.01	0.41
1:B:603:LYS:HE3	1:B:603:LYS:HB3	1.37	0.41
1:A:591:ALA:O	1:A:592:ALA:C	2.59	0.41
1:A:639:LEU:O	1:A:640:ASN:CB	2.68	0.41
1:A:680:ASP:OD1	1:A:682:HIS:CD2	2.64	0.41
1:B:611:ALA:HB3	1:B:758:ALA:CB	2.51	0.41
1:B:627:ARG:HH11	1:B:627:ARG:CG	2.31	0.41
1:A:753:VAL:HG22	1:A:754:THR:N	2.35	0.41
1:A:419:ARG:O	1:A:678:HIS:HD2	2.03	0.41
1:B:719:LEU:HD12	1:B:719:LEU:HA	1.85	0.41
1:B:659:GLU:HG2	1:B:681:ASN:O	2.21	0.40
1:B:389:LYS:O	1:B:589:ILE:HA	2.20	0.40
1:B:337:ASP:HB2	1:B:338:TYR:H	1.48	0.40
1:B:354:TYR:CE1	1:B:597:VAL:CG1	3.04	0.40
1:B:583:LYS:O	1:B:584:HIS:HB3	2.22	0.40
1:A:535:VAL:O	1:A:538:TYR:HB2	2.21	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:A:359:ASP:CB	1:A:411:TYR:CD2[3_645]	2.05	0.15

## 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	465/494 (94%)	399 (86%)	44 (10%)	22 (5%)	3	17
1	B	447/494 (90%)	388 (87%)	43 (10%)	16 (4%)	4	24
All	All	912/988 (92%)	787 (86%)	87 (10%)	38 (4%)	3	20

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	ASP
1	A	360	ASN
1	A	361	VAL
1	A	363	ALA
1	A	386	GLY
1	A	733	GLY
1	A	788	GLY
1	B	114	THR
1	B	376	ARG
1	B	593	ASP
1	B	743	GLY
1	B	744	LYS
1	A	364	LYS
1	A	505	GLY
1	A	532	GLY
1	A	742	GLU
1	A	744	LYS
1	B	358	ARG
1	B	412	LEU
1	B	442	ASN
1	B	505	GLY
1	B	741	VAL
1	A	490	PHE
1	B	444	GLN
1	B	594	GLY

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Mol	Chain	Res	Type
1	A	339	LEU
1	A	358	ARG
1	A	372	GLN
1	A	719	LEU
1	B	656	ASN
1	A	116	ILE
1	A	475	GLY
1	A	602	ASP
1	B	504	THR
1	B	788	GLY
1	A	487	PRO
1	B	733	GLY
1	A	387	GLY

### 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	386/409 (94%)	322 (83%)	64 (17%)	3	13
1	B	373/409 (91%)	310 (83%)	63 (17%)	2	13
All	All	759/818 (93%)	632 (83%)	127 (17%)	3	13

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	106	SER
1	A	107	GLU
1	A	108	ILE
1	A	355	LEU
1	A	358	ARG
1	A	359	ASP
1	A	360	ASN
1	A	364	LYS
1	A	365	GLU

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	367	LYS
1	A	368	ASN
1	A	377	ASP
1	A	381	LYS
1	A	385	ASN
1	A	395	ASP
1	A	397	LYS
1	A	404	SER
1	A	446	ASN
1	A	448	ASN
1	A	457	SER
1	A	465	LEU
1	A	479	SER
1	A	487	PRO
1	A	514	ASN
1	A	516	SER
1	A	526	ARG
1	A	548	GLU
1	A	561	GLU
1	A	585	VAL
1	A	588	LYS
1	A	596	VAL
1	A	597	VAL
1	A	601	GLN
1	A	610	LYS
1	A	615	ILE
1	A	617	GLN
1	A	622	GLU
1	A	625	SER
1	A	626	SER
1	A	633	LYS
1	A	638	SER
1	A	640	ASN
1	A	656	ASN
1	A	657	GLN
1	A	660	ASN
1	A	666	SER
1	A	687	GLN
1	A	691	SER
1	A	705	GLN
1	A	706	GLN

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Mol	Chain	Res	Type
1	A	711	ILE
1	A	719	LEU
1	A	727	GLU
1	A	728	VAL
1	A	738	LYS
1	A	745	GLU
1	A	748	VAL
1	A	754	THR
1	A	759	ASN
1	A	760	LYS
1	A	781	ASN
1	A	787	VAL
1	B	108	ILE
1	B	111	SER
1	B	116	ILE
1	B	119	ILE
1	B	120	GLU
1	B	343	THR
1	B	350	ARG
1	B	357	GLN
1	B	358	ARG
1	B	368	ASN
1	B	371	THR
1	B	372	GLN
1	B	376	ARG
1	B	377	ASP
1	B	389	LYS
1	B	391	THR
1	B	394	ILE
1	B	395	ASP
1	B	396	GLN
1	B	397	LYS
1	B	400	SER
1	B	428	ASP
1	B	430	GLN
1	B	444	GLN
1	B	457	SER
1	B	466	LEU
1	B	479	SER
1	B	502	LYS
1	B	516	SER
1	B	518	ASN

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Mol	Chain	Res	Type
1	B	545	GLU
1	B	552	GLU
1	B	585	VAL
1	B	590	GLU
1	B	593	ASP
1	B	597	VAL
1	B	603	LYS
1	B	619	LEU
1	B	630	THR
1	B	640	ASN
1	B	649	ILE
1	B	651	LYS
1	B	679	ASP
1	B	684	LEU
1	B	704	ILE
1	B	706	GLN
1	B	710	SER
1	B	711	ILE
1	B	719	LEU
1	B	727	GLU
1	B	739	VAL
1	B	740	SER
1	B	742	GLU
1	B	745	GLU
1	B	749	THR
1	B	752	THR
1	B	760	LYS
1	B	761	SER
1	B	769	ARG
1	B	772	ILE
1	B	779	TYR
1	B	780	GLN
1	B	784	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	368	ASN
1	A	399	HIS
1	A	485	ASN
1	A	494	ASN

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Mol	Chain	Res	Type
1	A	567	HIS
1	A	569	ASN
1	A	601	GLN
1	A	635	ASN
1	A	640	ASN
1	A	656	ASN
1	A	678	HIS
1	A	682	HIS
1	A	699	HIS
1	A	706	GLN
1	A	734	GLN
1	B	372	GLN
1	B	399	HIS
1	B	424	ASN
1	B	485	ASN
1	B	514	ASN
1	B	567	HIS
1	B	569	ASN
1	B	606	GLN
1	B	635	ASN
1	B	640	ASN
1	B	678	HIS
1	B	682	HIS
1	B	706	GLN
1	B	734	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
2	CEF	A	1460	1	18,27,31	3.03	7 (38%)	16,37,42	6.29	8 (50%)
3	SO4	A	1790	-	4,4,4	1.55	2 (50%)	6,6,6	0.95	0
2	CEF	B	1460	1	18,27,31	3.46	8 (44%)	16,37,42	6.93	7 (43%)
3	SO4	B	1790	-	4,4,4	0.87	0	6,6,6	1.18	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
2	CEF	A	1460	1	-	0/10/38/43	0/1/2/2
3	SO4	A	1790	-	-	0/0/0/0	0/0/0/0
2	CEF	B	1460	1	-	0/10/38/43	0/1/2/2
3	SO4	B	1790	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1460	CEF	C2-S1	-3.47	1.74	1.82
2	B	1460	CEF	O12-C11	-3.33	1.17	1.23
2	B	1460	CEF	C2-S1	-2.99	1.75	1.82
2	A	1460	CEF	C13-C11	-2.69	1.45	1.50
2	A	1460	CEF	C4'-C4	-2.54	1.47	1.52
2	B	1460	CEF	C13-C11	-2.42	1.46	1.50
3	A	1790	SO4	O4-S	2.04	1.54	1.47
3	A	1790	SO4	O2-S	2.26	1.54	1.47
2	A	1460	CEF	O17-N16	3.38	1.47	1.40
2	B	1460	CEF	O17-C18	4.05	1.49	1.43
2	B	1460	CEF	O17-N16	4.32	1.49	1.40
2	A	1460	CEF	O17-C18	4.43	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1460	CEF	C15-S16	4.68	1.78	1.70
2	B	1460	CEF	C3-C4	4.81	1.40	1.34
2	B	1460	CEF	C15-S16	5.83	1.79	1.70
2	A	1460	CEF	C13-N16	8.56	1.43	1.29
2	B	1460	CEF	C13-N16	9.51	1.45	1.29

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1460	CEF	O12-C11-C13	-12.02	107.12	120.53
2	A	1460	CEF	C3-C2-S1	-7.25	108.25	117.17
2	A	1460	CEF	O12-C11-C13	-6.30	113.50	120.53
2	B	1460	CEF	C3-C2-S1	-5.24	110.73	117.17
2	B	1460	CEF	C14-C15-S16	-3.78	107.14	111.79
2	A	1460	CEF	C14-C15-S16	-3.59	107.39	111.79
2	A	1460	CEF	N18-C17-N19	2.36	126.00	122.92
2	A	1460	CEF	C13-C11-N10	5.80	124.24	114.41
2	B	1460	CEF	C13-C11-N10	7.81	127.65	114.41
2	B	1460	CEF	O17-N16-C13	7.92	120.55	111.11
2	B	1460	CEF	C2-S1-C6	8.90	111.53	94.36
2	A	1460	CEF	C2-S1-C6	9.49	112.66	94.36
2	A	1460	CEF	O17-N16-C13	12.58	126.11	111.11
2	A	1460	CEF	C18-O17-N16	15.33	126.02	108.47
2	B	1460	CEF	C18-O17-N16	19.17	130.41	108.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1460	CEF	2	0
2	B	1460	CEF	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	469/494 (94%)	-0.59	2 (0%) 93 80	16, 35, 63, 85	0
1	B	455/494 (92%)	-0.56	1 (0%) 95 87	15, 31, 68, 87	0
All	All	924/988 (93%)	-0.58	3 (0%) 94 84	15, 33, 65, 87	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	2.4
1	B	743	GLY	2.1
1	A	780	GLN	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](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CEF	B	1460	26/30	0.97	0.18	1.60	31,39,44,54	0
2	CEF	A	1460	26/30	0.97	0.15	0.92	28,43,50,56	0
3	SO4	A	1790	5/5	0.97	0.13	-0.06	25,26,36,37	0
3	SO4	B	1790	5/5	0.98	0.12	-0.62	37,43,48,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.