

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 03:12 pm GMT

PDB ID	:	2XD1
Title	:	ACTIVE SITE RESTRUCTURING REGULATES LIGAND RECOGNI-
		TION IN CLASS A PENICILLIN-BINDING PROTEINS
Authors	:	Macheboeuf, P.; Di Guilmi, A.M.; Job, V.; Vernet, T.; Dideberg, O.; Dessen,
		А.
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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	494	46%	37%	11% • 5%		
1	В	494	45%	34%	11% • 8%		



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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	460	Total	С	Ν	0	S	0	0	0
		409	3617	2263	613	726	15	0	0	0
1	р	455	Total	С	Ν	0	S	0	0	0
	I D	400	3508	2195	594	704	15	0	0	0

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	686	GLN	ARG	engineered mutation	UNP Q7CRA4
А	687	GLN	ARG	engineered mutation	UNP Q7CRA4
В	686	GLN	ARG	engineered mutation	UNP Q7CRA4
В	687	GLN	ARG	engineered mutation	UNP Q7CRA4

• Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (three-letter code: CEF) (formula: $C_{14}H_{15}N_5O_5S_2$).





Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf
2	Λ	1	Total	С	Ν	0	\mathbf{S}	0	0
		1	26	14	5	5	2	0	0
0	В	1	Total	С	Ν	0	S	0	0
	D	1	26	14	5	5	2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	44	Total O 44 44	0	0
4	В	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0



3 Residue-property plots (i)

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 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



E540 K541 M542 M542 **G543** Y544 E545 E545 I546 K583 H584 V585 I586 A611 T612 A613 R526 <mark>8625</mark> L619 L620 R621 E622 1554 2555 1617 H699 L700 3626 3627 D679 D680 N681 H682 S683 S683 L684 L684 S685 1630 N640 P641 r642 .643 .644 4644 N645 3666 1661 1667 67 S755 Y756 W757 A758 A758 A759 N759 S761 G762 G762 A765 Y768 Y768 R769 R769 R771 D778 V701 E727 <mark>V728</mark> L729 F717



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	96.60Å 102.30Å 146.50Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution(A)	45.22 - 3.00	Depositor
Resolution (A)	45.20 - 3.00	EDS
% Data completeness	99.7 (45.22-3.00)	Depositor
(in resolution range)	99.7 (45.20-3.00)	EDS
R_{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.74 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.161 , 0.248	Depositor
II, II, <i>free</i>	0.163 , 0.247	DCC
R_{free} test set	2955 reflections $(9.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	46.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 46.4	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7278	wwPDB-VP
Average B, all atoms $(Å^2)$	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.

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



¹Intensities estimated from amplitudes.

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: SO4, CEF

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).

Mal	Chain	Bo	nd lengths	Bond angles		
INIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.62	38/3690~(1.0%)	1.48	36/5009~(0.7%)	
1	В	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	А	0	2
1	В	0	4
All	All	0	6

All (83) bond length outliers are listed below:

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



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



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

Continued from previous page...

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	460	SER	O-C-N	-13.25	101.50	122.70
1	А	428	ASP	CB-CG-OD1	9.71	127.04	118.30
1	В	395	ASP	CB-CG-OD2	9.40	126.76	118.30
1	А	395	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	А	459	ALA	O-C-N	-9.39	107.68	122.70
1	А	395	ASP	CB-CG-OD1	8.31	125.78	118.30
1	В	459	ALA	CA-C-N	-8.22	99.11	117.20
1	В	526	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	А	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	В	546	ILE	C-N-CD	7.75	144.68	128.40



2X	D1

Mol	Chain	Res	Tvpe	Atoms	Z	$Observed(^{o})$	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	В	729	LEU	CA-CB-CG	6.83	131.02	115.30
1	В	114	THR	N-CA-CB	6.80	123.23	110.30
1	А	373	LYS	CD-CE-NZ	-6.79	96.09	111.70
1	В	395	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	А	574	LEU	CB-CG-CD1	-6.63	99.73	111.00
1	В	762	GLY	N-CA-C	-6.62	96.54	113.10
1	А	717	PHE	N-CA-C	-6.46	93.56	111.00
1	В	113	GLY	N-CA-C	-6.46	96.96	113.10
1	А	735	LYS	CD-CE-NZ	-6.38	97.03	111.70
1	В	679	ASP	CB-CG-OD1	6.35	124.02	118.30
1	А	556	MET	CG-SD-CE	-6.35	90.04	100.20
1	А	414	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	А	504	THR	C-N-CA	-6.30	109.08	122.30
1	В	590	GLU	N-CA-CB	6.27	121.88	110.60
1	В	419	ARG	CG-CD-NE	-6.18	98.81	111.80
1	А	337	ASP	CB-CG-OD2	6.15	123.84	118.30
1	А	358	ARG	N-CA-C	-6.06	94.64	111.00
1	В	350	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	В	375	TYR	CA-CB-CG	-6.04	101.92	113.40
1	В	554	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	В	526	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	В	506	MET	CB-CA-C	-5.88	98.65	110.40
1	В	502	LYS	CD-CE-NZ	-5.87	98.20	111.70
1	В	436	GLY	N-CA-C	-5.87	98.43	113.10
1	А	428	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	В	455	LYS	CD-CE-NZ	-5.83	98.28	111.70
1	В	526	ARG	CG-CD-NE	5.80	123.97	111.80
1	А	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	В	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



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	397	LYS	CD-CE-NZ	-5.43	99.20	111.70
1	А	627	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	А	358	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	В	402	MET	CG-SD-CE	5.32	108.70	100.20
1	А	667	THR	C-N-CD	5.31	139.54	128.40
1	В	505	GLY	N-CA-C	5.30	126.35	113.10
1	В	636	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	А	625	SER	CA-CB-OG	-5.29	96.93	111.20
1	В	386	GLY	N-CA-C	5.27	126.27	113.10
1	В	750	GLY	N-CA-C	-5.24	100.00	113.10
1	А	751	SER	N-CA-CB	5.22	118.34	110.50
1	В	444	GLN	N-CA-CB	-5.20	101.24	110.60
1	В	378	LEU	CB-CG-CD1	5.16	119.76	111.00
1	А	669	ARG	CB-CG-CD	-5.12	98.27	111.60
1	В	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	А	359	ASP	Peptide
1	А	460	SER	Mainchain
1	В	371	THR	Peptide
1	В	375	TYR	Peptide
1	В	459	ALA	Mainchain
1	В	666	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3617	0	3484	161	1
1	В	3508	0	3363	189	0
2	А	26	0	0	2	0
2	В	26	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	5	0	0	0	0
3	В	5	0	0	0	0
4	А	44	0	0	3	0
4	В	47	0	0	6	0
All	All	7278	0	6847	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	Clash
Atom-1	Atom-2	distance (\AA)	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:HA	1:B:706:GLN:NE2	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:HA	1:A:687:GLN:OE1	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:376:ARG:HD3	4:A:2005:HOH:O	1.68	0.93
1:A:643:LEU:HD22	1:A:705:GLN:HG2	1.50	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:O3	1.70	0.90
1:B:706:GLN:HA	1:B:706:GLN:HE21	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:OE1	1:A:687:GLN:CA	2.29	0.81
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.47	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:C	1:A:640:ASN:HD22	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:CD	1:A:715:GLU:H	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: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:377:ASP:C	1:B:377:ASP:OD2	2.31	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:337:ASP:HA	4:B:2004:HOH:O	1.92	0.68
1:B:376:ARG:CG	1:B:377:ASP:N	2.56	0.68
1:A:745:GLU:O	1:A:745:GLU:HG3	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:385:ASN:O	1:A:387:GLY:N	2.28	0.66
1:A:739:VAL:HG12	1:A:740:SER:N	2.09	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



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:611:ALA:O	1:B:615:ILE:HG13	1.98	0.64
1:B:706:GLN:HE21	1:B:706:GLN:N	1.94	0.64
1:A:621:ARG:HB2	1:A:649:ILE:HG22	1.78	0.64
1:A:643:LEU:HD22	1:A:705:GLN:HG3	1.77	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:A:544:TYR:OH	1:A:567:HIS:HD2	1.80	0.63
1:B:380:ALA:O	1:B:386:GLY:CA	2.47	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:A:760:LYS:H	1:A:760:LYS:HD3	1.63	0.62
1:B:358:ARG:O	1:B:359:ASP:C	2.38	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:A:368:ASN:HD21	1:A:371:THR:H	1.48	0.61
1:B:116:ILE:HD12	1:B:116:ILE:O	2.01	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:O	1:B:741:VAL:CG1	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:461:THR:OG1	1:B:567:HIS:HE1	1.86	0.59
1:B:739:VAL:HG23	1:B:748:VAL:HG23	1.85	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:A:738:LYS:HD2	1:A:747:GLU:OE2	2.04	0.57
1:B:640:ASN:ND2	1:B:643:LEU:H	2.02	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:596:VAL:HG12	1:A:596:VAL:O	2.05	0.57
1:A:728:VAL:HG12	1:A:734:GLN:C	2.24	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:A:632:PHE:HA	1:A:635:ASN:HD22	1.69	0.55
1:B:108:ILE:CG2	1:B:116:ILE:HG23	2.33	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:A:760:LYS:HG2	1:A:761:SER:N	2.22	0.55
1:B:358:ARG:HH11	1:B:358:ARG:CB	2.20	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:O3	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:525:TYR:HB2	1:A:555:PRO:HG3	1.90	0.53



		Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:780:GLN:O	1:A:784:SER:HB2	2.09	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:A:399:HIS:O	1:A:403:GLN:HG2	2.08	0.52	
1:B:108:ILE:CD1	1:B:343:THR:HG23	2.39	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:358:ARG:HH11	1:B:358:ARG:HB3	1.72	0.52	
1:B:688:ALA:HA	1:B:692:ASN:HB2	1.92	0.52	
1:A:468:TYR:O	1:A:469:GLY:C	2.48	0.52	
1:B:417:THR:HG21	1:B:683:SER:O	2.10	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:B:734:GLN:NE2	1:B:770:PHE:HB2	2.24	0.52	
1:A:489:ASN:OD1	1:A:495:PRO:HA	2.08	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:B:108:ILE:HG21	1:B:343:THR:HG21	1.92	0.52	
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.74	0.51	
1:A:459:ALA:CB	1:A:460:SER:N	2.73	0.51	
1:A:665:LEU:O	1:A:671:THR:HG23	2.10	0.51	
1:A:446:ASN:C	1:A:446:ASN:OD1	2.48	0.51	
1:A:472:ILE:HA	1:A:477:MET:O	2.10	0.51	
1:A:504:THR:O	1:A:505:GLY:C	2.48	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:376:ARG:O	1:A:379:ALA:HB3	2.12	0.50	



		Interatomic	Clash
Atom-2		distance (\AA)	overlap (Å)
1:A:460:SER:N	2:A:1460:CEF:O3	2.45	0.50
1:A:760:LYS:H	1:A:760:LYS:CD	2.24	0.50
1:B:375:TYR:N	1:B:375:TYR:HD1	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: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:B:339:LEU:O	1:B:343:THR:HB	2.12	0.50
1:A:358:ARG:NH1	1:A:360:ASN:OD1	2.45	0.49
1:A:643:LEU:CD2	1:A:705:GLN:HG2	2.33	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:446:ASN:OD1	1:B:446:ASN:C	2.50	0.49
1:B:622:GLU:HB3	4:B:2028:HOH:O	2.11	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:376:ARG:HG3	1:B:377:ASP:H	1.71	0.49
1:B:449:ASN:O	1:B:453:ASP:HB2	2.11	0.49
1:A:399:HIS:CD2	1:A:437:PHE:H	2.31	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:487:PRO:O	1:A:488:THR:HB	2.12	0.49
1:B:654:THR:HG23	1:B:661:MET:SD	2.52	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:A:620:LEU:HA	1:A:620:LEU:HD23	1.57	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:B:768:TYR:CE2	1:B:783:TRP:CD1	3.01	0.48
1:B:486:TYR:CE1	1:B:505:GLY:HA2	2.48	0.48
1:B:734:GLN:HB2	1:B:766:THR:HA	1.96	0.48
1:B:734:GLN:HE22	1:B:770:PHE:CB	2.27	0.48
1:A:485:ASN:HB3	1:A:507:MET:CE	2.44	0.47
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



		Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:A:487:PRO:HG3	1:A:502:LYS:O	2.15	0.47
1:A:528:LEU:HD22	1:A:533:VAL:HG21	1.96	0.47
1:A:715:GLU:CD	1:A:715:GLU:N	2.64	0.47
1:B:784:SER:OG	1:B:785:SER:N	2.47	0.47
1:A:523:TRP:CG	1:A:773:GLY:HA3	2.49	0.47
1:A:760:LYS:HG2	1:A:761:SER:H	1.79	0.47
1:B:403:GLN:HA	1:B:403:GLN:HE21	1.80	0.47
1:A:112:ASP:OD1	1:A:113:GLY:N	2.48	0.47
1:B:357:GLN:C	1:B:358:ARG:O	2.53	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: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:A:462:THR:HB	1:A:555:PRO:O	2.16	0.46
1:A:569:ASN:HD21	1:A:583:LYS:H	1.62	0.46
1:B:376:ARG:HG3	1:B:377:ASP:HB3	1.97	0.46
1:B:783:TRP:O	1:B:784:SER:C	2.53	0.46
1:A:473:ASP:HA	1:A:612:THR:OG1	2.15	0.46
1:B:108:ILE:O	1:B:116:ILE:N	2.43	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:B:473:ASP:HB2	1:B:612:THR:HG21	1.96	0.46
1:A:738:LYS:HA	1:A:746:VAL:O	2.15	0.46
1:A:739:VAL:CG1	1:A:740:SER:N	2.78	0.46
1:B:729:LEU:CD2	1:B:736:PRO:HB3	2.42	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:A:357:GLN:O	1:A:359:ASP:N	2.49	0.45
1:B:740:SER:O	1:B:742:GLU: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:A:554:LEU:HD12	1:A:558:GLY:O	2.17	0.45
1:B:375:TYR:O	1:B:377:ASP:N	2.50	0.45
1:B:735:LYS:HB2	1:B:765:ALA:HA	1.98	0.45
1:B:760:LYS:H	1:B:760:LYS:CD	2.30	0.45



	i agem	Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:B:780:GLN:HG3	1:B:781:ASN:N	2.20	0.45
1:A:350:ARG:HG2	1:A:350:ARG:NH1	2.32	0.45
1:A:455:LYS:HA	1:A:562:VAL:O	2.17	0.45
1:B:487:PRO:O	1:B:488:THR:HB	2.17	0.45
1:A:615:ILE:HD11	1:A:723:VAL:HG13	1.99	0.45
1:A:498:TYR:CD1	1:A:517:TRP:HA	2.52	0.45
1:B:661:MET:HB2	1:B:676:ILE:HG12	1.99	0.45
1:A:569:ASN:ND2	1:A:583:LYS:H	2.15	0.45
1:A:615:ILE:HD13	1:A:756:TYR:CB	2.47	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:A:640:ASN:HD21	1:A:643:LEU:H	1.64	0.44
1:B:116:ILE:HG12	1:B:339:LEU:HG	1.99	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:A:671:THR:HG22	1:A:672:LEU:N	2.33	0.44
1:B:485:ASN:ND2	1:B:519:ILE:HB	2.33	0.44
1:A:596:VAL:O	1:A:596:VAL:CG1	2.66	0.43
1:A:612:THR:HG22	1:A:613:ALA:N	2.32	0.43
1:A:723:VAL:HG12	1:A:724:VAL:N	2.34	0.43
1:A:503:GLY:C	1:A:504:THR:HG23	2.39	0.43
1:B:706:GLN:NE2	1:B:706:GLN:CA	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:521:ALA:O	1:B:555:PRO:HG2	2.19	0.43
1:B:734:GLN:NE2	1:B:770:PHE:CB	2.82	0.43
1:A:459:ALA:CA	1:A:460:SER:N	2.73	0.43
1:A:671:THR:CG2	1:A:672:LEU:N	2.82	0.43
1:A:728:VAL:HG21	1:A:755:SER:HB2	2.00	0.43
1:A:454:THR:O	1:A:563:THR:HG22	2.19	0.42
1:A:391:THR:HG22	1:A:587:SER:OG	2.19	0.42
1:A:485:ASN:ND2	1:A:519:ILE:HB	2.34	0.42
1:B:372:GLN:HE21	1:B:372:GLN:HB3	1.65	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:B:446:ASN:OD1	1:B:447:GLN:N	2.53	0.42
1:B:352:TYR:CD2	1:B:352:TYR:C	2.92	0.42



		Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:613:ALA:O	1:A:617:GLN:HG2	2.19	0.42	
1:B:542:MET:HA	1:B:580:TYR:CD1	2.54	0.42	
1:B:424:ASN:HA	1:B:673:GLY:O	2.20	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:643:LEU:C	1:A:645:ASN:N	2.70	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:CD1	1:B:437:PHE:C	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:480:GLU:HB2	1:B:755:SER:HB2	2.03	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:A:591:ALA:O	1:A:592:ALA:C	2.59	0.41	
1:B:603:LYS:HB3	1:B:603:LYS:HE3	1.37	0.41	
1:B:622:GLU:HA	1:B:625:SER:HB2	2.01	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:A:753:VAL:HG22	1:A:754:THR:N	2.35	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: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:A:535:VAL:O	1:A:538:TYR:HB2	2.21	0.40	
1:B:583:LYS:O	1:B:584:HIS:HB3	2.22	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 (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	А	465/494~(94%)	399~(86%)	44 (10%)	22~(5%)	2 14
1	В	447/494~(90%)	388 (87%)	43 (10%)	16 (4%)	3 19
All	All	912/988~(92%)	787~(86%)	87 (10%)	38~(4%)	3 16

All (38) Ramachandran outliers are listed below:

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



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

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	А	386/409~(94%)	322~(83%)	64 (17%)	2 11
1	В	373/409~(91%)	310~(83%)	63~(17%)	2 11
All	All	759/818~(93%)	632(83%)	127 (17%)	2 11

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

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



1 A 366 LEU 1 A 367 LYS 1 A 367 LYS 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 404 SER 1 A 446 ASN 1 A 446 SN 1 A 446 SN 1 A 446 SN 1 A 446 SN 1 A 446 ASN 1 A 446 ASN 1 A 457 SER 1 A 514 ASN 1 A 516 SER 1 A 561 GLU 1 A 561 GLU	Mol	Chain	Res	Type
1 A 367 LYS 1 A 368 ASN 1 A 377 ASP 1 A 381 LYS 1 A 395 ASN 1 A 395 ASP 1 A 397 LYS 1 A 404 SER 1 A 404 SER 1 A 446 ASN 1 A 446 SSN 1 A 446 SSN 1 A 446 SSN 1 A 446 SSN 1 A 457 SER 1 A 465 LEU 1 A 516 SER 1 A 516 SER 1 A 516 GLU 1 A 561 GLU 1 A 597 VAL 1 A 615 ILE <td>1</td> <td>А</td> <td>366</td> <td>LEU</td>	1	А	366	LEU
1 A 368 ASN 1 A 377 ASP 1 A 381 LYS 1 A 395 ASN 1 A 395 ASP 1 A 395 ASP 1 A 397 LYS 1 A 404 SER 1 A 446 ASN 1 A 446 ASN 1 A 446 SER 1 A 446 ASN 1 A 447 SER 1 A 457 SER 1 A 465 LEU 1 A 514 ASN 1 A 516 SER 1 A 516 GLU 1 A 561 GLU 1 A 585 VAL 1 A 597 VAL 1 A 610 LYS <td>1</td> <td>А</td> <td>367</td> <td>LYS</td>	1	А	367	LYS
1 A 377 ASP 1 A 381 LYS 1 A 395 ASN 1 A 395 ASP 1 A 397 LYS 1 A 404 SER 1 A 404 SER 1 A 446 ASN 1 A 446 ASN 1 A 4479 SER 1 A 479 SER 1 A 479 SER 1 A 516 SER 1 A 516 SER 1 A 561 GLU 1 A 561 GLU 1 A 561 GLU 1 A 588 LYS 1 A 597 VAL 1 A 610 LYS 1 A 610 LYS 1 A 625 SER </td <td>1</td> <td>А</td> <td>368</td> <td>ASN</td>	1	А	368	ASN
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 446 ASN 1 A 446 ASN 1 A 4479 SER 1 A 465 LEU 1 A 479 SER 1 A 479 SER 1 A 516 SER 1 A 516 SER 1 A 561 GLU 1 A 585 VAL 1 A 588 LYS 1 A 601 GLN 1 A 615 ILE 1 A 615 ILE 1 A 626	1	А	377	ASP
1 A 385 ASN 1 A 395 ASP 1 A 397 LYS 1 A 404 SER 1 A 446 ASN 1 A 446 ASN 1 A 446 ASN 1 A 447 SER 1 A 465 LEU 1 A 467 PRO 1 A 479 SER 1 A 514 ASN 1 A 516 SER 1 A 561 GLU 1 A 563 VAL 1 A 585 VAL 1 A 596 VAL 1 A 610 LYS 1 A 615 ILE 1 A 615 ILE 1 A 626 SER 1 A 626 SER 1	1	А	381	LYS
1 A 395 ASP 1 A 397 LYS 1 A 404 SER 1 A 446 ASN 1 A 446 ASN 1 A 446 ASN 1 A 447 SER 1 A 465 LEU 1 A 479 SER 1 A 479 SER 1 A 514 ASN 1 A 516 SER 1 A 526 ARG 1 A 561 GLU 1 A 561 GLU 1 A 585 VAL 1 A 596 VAL 1 A 610 LYS 1 A 610 LYS 1 A 617 GLN 1 A 617 GLN 1 A 625 SER <td>1</td> <td>А</td> <td>385</td> <td>ASN</td>	1	А	385	ASN
1 A 397 LYS 1 A 404 SER 1 A 446 ASN 1 A 446 ASN 1 A 4457 SER 1 A 457 SER 1 A 465 LEU 1 A 479 SER 1 A 479 SER 1 A 514 ASN 1 A 516 SER 1 A 526 ARG 1 A 561 GLU 1 A 585 VAL 1 A 585 VAL 1 A 597 VAL 1 A 610 LYS 1 A 610 LYS 1 A 610 LYS 1 A 622 GLU 1 A 625 SER 1 A 626 SER 1	1	А	395	ASP
1 A 404 SER 1 A 446 ASN 1 A 4457 SER 1 A 457 SER 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 561 GLU 1 A 585 VAL 1 A 588 LYS 1 A 596 VAL 1 A 597 VAL 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	1	А	397	LYS
1 A 446 ASN 1 A 448 ASN 1 A 457 SER 1 A 465 LEU 1 A 479 SER 1 A 479 SER 1 A 487 PRO 1 A 514 ASN 1 A 516 SER 1 A 526 ARG 1 A 561 GLU 1 A 588 LYS 1 A 588 LYS 1 A 596 VAL 1 A 597 VAL 1 A 610 LYS 1 A 615 ILE 1 A 615 ILE 1 A 622 GLU 1 A 625 SER 1 A 626 SER 1 A 633 LYS 1	1	А	404	SER
1 A 448 ASN 1 A 457 SER 1 A 465 LEU 1 A 479 SER 1 A 479 SER 1 A 487 PRO 1 A 514 ASN 1 A 516 SER 1 A 526 ARG 1 A 561 GLU 1 A 563 VAL 1 A 585 VAL 1 A 596 VAL 1 A 597 VAL 1 A 610 LYS 1 A 610 LYS 1 A 615 ILE 1 A 617 GLN 1 A 625 SER 1 A 626 SER 1 A 633 LYS 1 A 638 SER 1	1	А	446	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 561 GLU 1 A 563 VAL 1 A 585 VAL 1 A 596 VAL 1 A 597 VAL 1 A 601 GLN 1 A 615 ILE 1 A 615 ILE 1 A 617 GLN 1 A 622 GLU 1 A 626 SER 1 A 626 SER 1 A 626 SER 1 A 638 SER 1 A 638 SER 1	1	А	448	ASN
1 A 465 LEU 1 A 479 SER 1 A 514 ASN 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 615 ILE 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 640 ASN 1 A 656 ASN 1	1	А	457	SER
1 A 479 SER 1 A 487 PRO 1 A 514 ASN 1 A 516 SER 1 A 526 ARG 1 A 526 ARG 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 625 SER 1 A 626 SER 1 A 633 LYS 1 A 636 ASN 1 A 656 ASN 1	1	А	465	LEU
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 615 ILE 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 666 SER 1	1	А	479	SER
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 656 ASN 1 A 657 GLN 1 A 656 ASN 1 A 666 SER 1	1	А	487	PRO
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 656 ASN 1 A 657 GLN 1 A 656 ASN 1 A 666 SER 1 A 666 SER 1	1	А	514	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	516	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	526	ARG
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	561	GLU
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	588	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	596	VAL
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	601	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	610	LYS
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 638 SER 1 A 656 ASN 1 A 656 ASN 1 A 656 SER 1 A 656 SEN 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	615	ILE
1 A 622 GLU 1 A 625 SER 1 A 626 SER 1 A 633 LYS 1 A 633 LYS 1 A 638 SER 1 A 638 SER 1 A 656 ASN 1 A 656 ASN 1 A 656 SER 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	617	GLN
1 A 625 SER 1 A 626 SER 1 A 633 LYS 1 A 638 SER 1 A 638 SER 1 A 636 ASN 1 A 656 ASN 1 A 657 GLN 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 667 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	622	GLU
1 A 626 SER 1 A 633 LYS 1 A 638 SER 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 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	625	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 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	626	SER
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 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	633	LYS
1 A 640 ASN 1 A 656 ASN 1 A 657 GLN 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	638	SER
1 A 656 ASN 1 A 657 GLN 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	640	ASN
1 A 657 GLN 1 A 660 ASN 1 A 666 SER 1 A 666 SER 1 A 667 GLN 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	A	656	ASN
1 A 660 ASN 1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	657	GLN
1 A 666 SER 1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	660	ASN
1 A 687 GLN 1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	A	666	SER
1 A 691 SER 1 A 705 GLN 1 A 706 GLN	1	А	687	GLN
1 A 705 GLN 1 A 706 GLN	1	А	691	SER
1 A 706 GLN	1	А	705	GLN
	1	A	706	GLN



	e
1 A 711 ILE	E
1 A 719 LE	IJ
1 A 727 GL	U
1 A 728 VA	L
1 A 738 LYS	S
1 A 745 GL	U
1 A 748 VA	L
1 A 754 TH	R
1 A 759 ASI	N
1 A 760 LYS	S
1 A 781 ASI	N
1 A 787 VA	L
1 B 108 ILE	E
1 B 111 SEI	R
1 B 116 ILE	E
1 B 119 ILE	E
1 B 120 GL	U
1 B 343 TH	R
1 B 350 AR	G
1 B 357 GL	N
1 B 358 AR	G
1 B 368 ASI	N
1 B 371 TH	R
1 B 372 GL	N
1 B 376 AR	G
1 B 377 AS	P
1 B 389 LYS	S
1 B 391 TH	R
1 B 394 ILE	E
1 B 395 AS	P
1 B 396 GL	N
1 B 397 LYS	S
1 B 400 SEI	R
1 B 428 AS	P
1 B 430 GL	N
1 B 444 GL	N
1 B 457 SEI	R
1 B 466 LE	U
1 B 479 SEI	R
1 B 502 LYS	S
1 B 516 SEI	R
1 B 518 ASI	N



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

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

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



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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

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).

Mal	Turne	Chain	Dec	Tinle	B	ond leng	gths	B	ond ang	les
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	CEF	А	1460	1	$19,\!27,\!27$	3.52	9 (47%)	14,37,37	6.50	7 (50%)
2	CEF	В	1460	1	19,27,27	4.04	10 (52%)	14,37,37	7.17	6 (42%)
3	SO4	А	1790	-	4,4,4	0.95	0	6,6,6	1.17	0
3	SO4	В	1790	-	4,4,4	0.58	0	6,6,6	1.35	1 (16%)

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	А	1460	1	-	3/14/38/38	0/1/2/2
2	CEF	В	1460	1	-	8/14/38/38	0/1/2/2

All (19)	bond	length	outliers	are	listed	below:	

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1460	CEF	C10-N3	10.14	1.45	1.29
2	В	1460	CEF	C3-C2	9.41	1.52	1.32
2	А	1460	CEF	C10-N3	9.12	1.43	1.29
2	А	1460	CEF	C3-C2	7.21	1.47	1.32
2	В	1460	CEF	C13-S2	5.83	1.79	1.70
2	А	1460	CEF	C13-S2	4.68	1.78	1.70
2	А	1460	CEF	O5-C11	4.30	1.50	1.43
2	В	1460	CEF	C4-N1	4.01	1.38	1.28
2	В	1460	CEF	O5-C11	3.93	1.49	1.43
2	В	1460	CEF	O5-N3	3.83	1.49	1.40
2	А	1460	CEF	C1-S1	-3.56	1.74	1.82
2	В	1460	CEF	O4-C9	-3.34	1.17	1.23
2	А	1460	CEF	C4-N1	3.26	1.36	1.28



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	1460	CEF	C4-C2	-3.25	1.35	1.46
2	В	1460	CEF	C1-S1	-3.06	1.75	1.82
2	А	1460	CEF	O5-N3	2.99	1.47	1.40
2	А	1460	CEF	C10-C9	-2.72	1.45	1.50
2	В	1460	CEF	C10-C9	-2.45	1.46	1.50
2	В	1460	CEF	O1-C5	2.28	1.28	1.22

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1460	CEF	C11-O5-N3	18.95	130.41	108.40
2	А	1460	CEF	C11-O5-N3	15.17	126.02	108.40
2	А	1460	CEF	O5-N3-C10	13.47	126.11	111.28
2	В	1460	CEF	O4-C9-C10	-11.48	107.12	120.35
2	А	1460	CEF	C1-S1-C6	9.27	112.66	94.47
2	В	1460	CEF	C1-S1-C6	8.70	111.53	94.47
2	В	1460	CEF	O5-N3-C10	8.42	120.55	111.28
2	В	1460	CEF	C10-C9-N2	7.99	127.65	114.38
2	А	1460	CEF	O4-C9-C10	-5.94	113.50	120.35
2	А	1460	CEF	C10-C9-N2	5.93	124.24	114.38
2	В	1460	CEF	C12-C13-S2	-3.78	107.14	111.79
2	A	1460	CEF	C12-C13-S2	-3.59	107.39	111.79
3	В	1790	SO4	O3-S-O2	-2.84	94.47	109.31
2	A	1460	CEF	N4-C14-N5	2.18	126.00	123.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1460	CEF	C9-C10-N3-O5
2	В	1460	CEF	C9-C10-N3-O5
2	В	1460	CEF	C10-N3-O5-C11
2	В	1460	CEF	N3-C10-C9-O4
2	А	1460	CEF	N3-C10-C9-N2
2	В	1460	CEF	N3-C10-C9-N2
2	В	1460	CEF	C12-C10-N3-O5
2	В	1460	CEF	N1-C4-C5-O2
2	В	1460	CEF	C2-C4-C5-O1
2	A	1460	CEF	N3-C10-C9-O4
2	В	1460	CEF	C12-C10-C9-O4

There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1460	CEF	2	0
2	В	1460	CEF	1	0

2 monomers are involved in 3 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	А	1
1	В	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	459:ALA	С	460:SER	N	1.70



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	502:LYS	С	503:GLY	Ν	1.62



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^{th} 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		$OWAB(Å^2)$	Q<0.9	
1	А	469/494~(94%)	-0.60	1 (0%)	95	87	16, 35, 63, 85	0
1	В	455/494~(92%)	-0.57	1 (0%)	95	87	15, 31, 68, 87	0
All	All	924/988~(93%)	-0.59	2(0%)	95	87	15, 33, 65, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	359	ASP	2.4
1	В	743	GLY	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	CEF	А	1460	26/26	0.97	0.15	$28,\!43,\!50,\!56$	0
2	CEF	В	1460	26/26	0.97	0.18	31,39,44,54	0
3	SO4	А	1790	5/5	0.97	0.13	25,26,36,37	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	SO4	В	1790	5/5	0.98	0.12	37,43,48,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

