



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 3QLB / pdb_00003qlb
Title : Enantiopyochelin outer membrane TonB-dependent transporter from *Pseudomonas fluorescens* bound to the ferri-enantiopyochelin
Authors : Brillet, K.; Noel, S.; Mislin, G.L.A.; Reimann, C.; Schalk, I.J.; Cobessi, D.
Deposited on : 2011-02-02
Resolution : 3.26 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

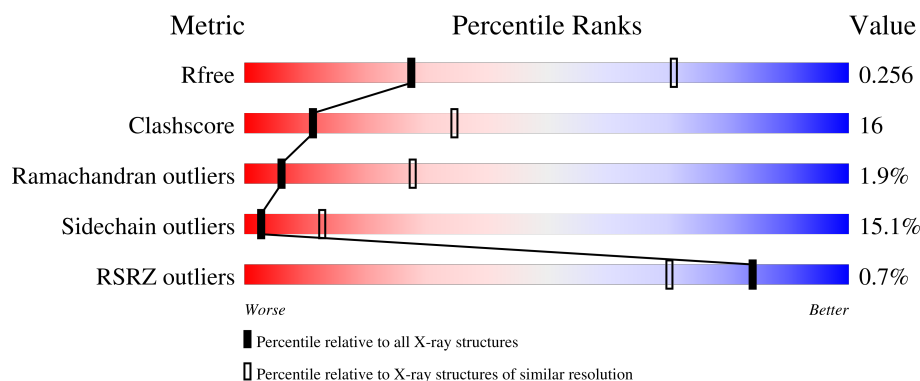
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 $\leq 5\%$. 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	748	55% 28% 6% 10%
1	B	748	53% 28% 8% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	A	700	-	X	-	-
3	CIT	B	700	-	X	X	-
4	EFE	A	701	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10529 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.

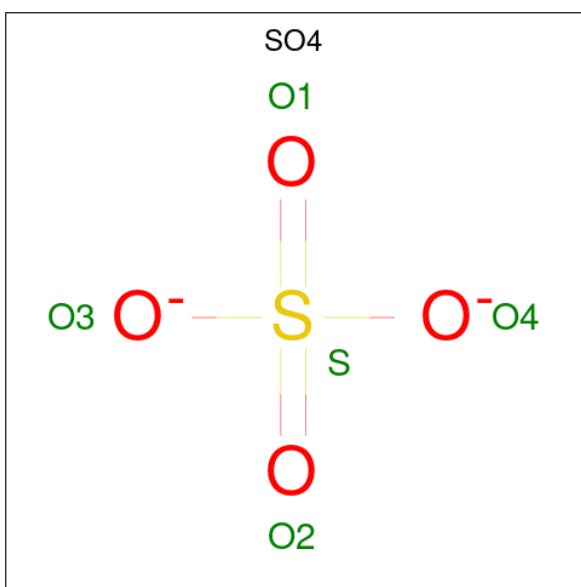
- Molecule 1 is a protein called Enantio-pyochelin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5235	3273	920	1034	8			
1	B	670	Total	C	N	O	S	0	0	0
			5214	3260	915	1031	8			

There are 10 discrepancies between the modelled and reference sequences:

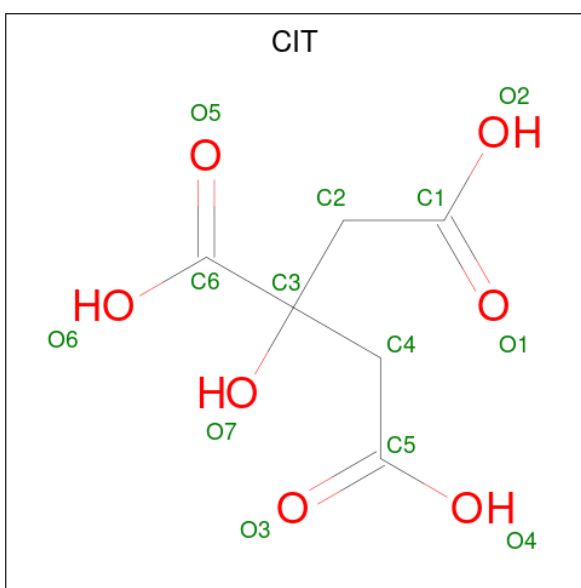
Chain	Residue	Modelled	Actual	Comment	Reference
A	388	HIS	-	SEE REMARK 999	UNP C5I2D9
A	389	HIS	-	SEE REMARK 999	UNP C5I2D9
A	390	HIS	-	SEE REMARK 999	UNP C5I2D9
A	391	HIS	-	SEE REMARK 999	UNP C5I2D9
A	392	HIS	-	SEE REMARK 999	UNP C5I2D9
B	388	HIS	-	SEE REMARK 999	UNP C5I2D9
B	389	HIS	-	SEE REMARK 999	UNP C5I2D9
B	390	HIS	-	SEE REMARK 999	UNP C5I2D9
B	391	HIS	-	SEE REMARK 999	UNP C5I2D9
B	392	HIS	-	SEE REMARK 999	UNP C5I2D9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



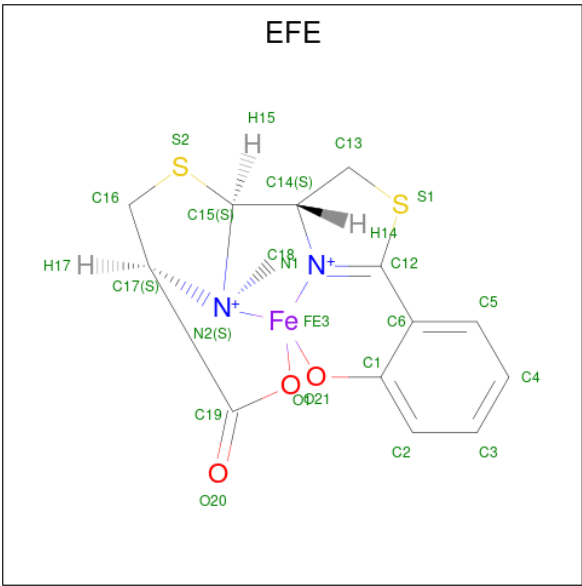
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ENANTIO-PYOCHELIN FE(III) (CCD ID: EFE) (formula: C₁₄H₁₄FeN₂O₃S₂).

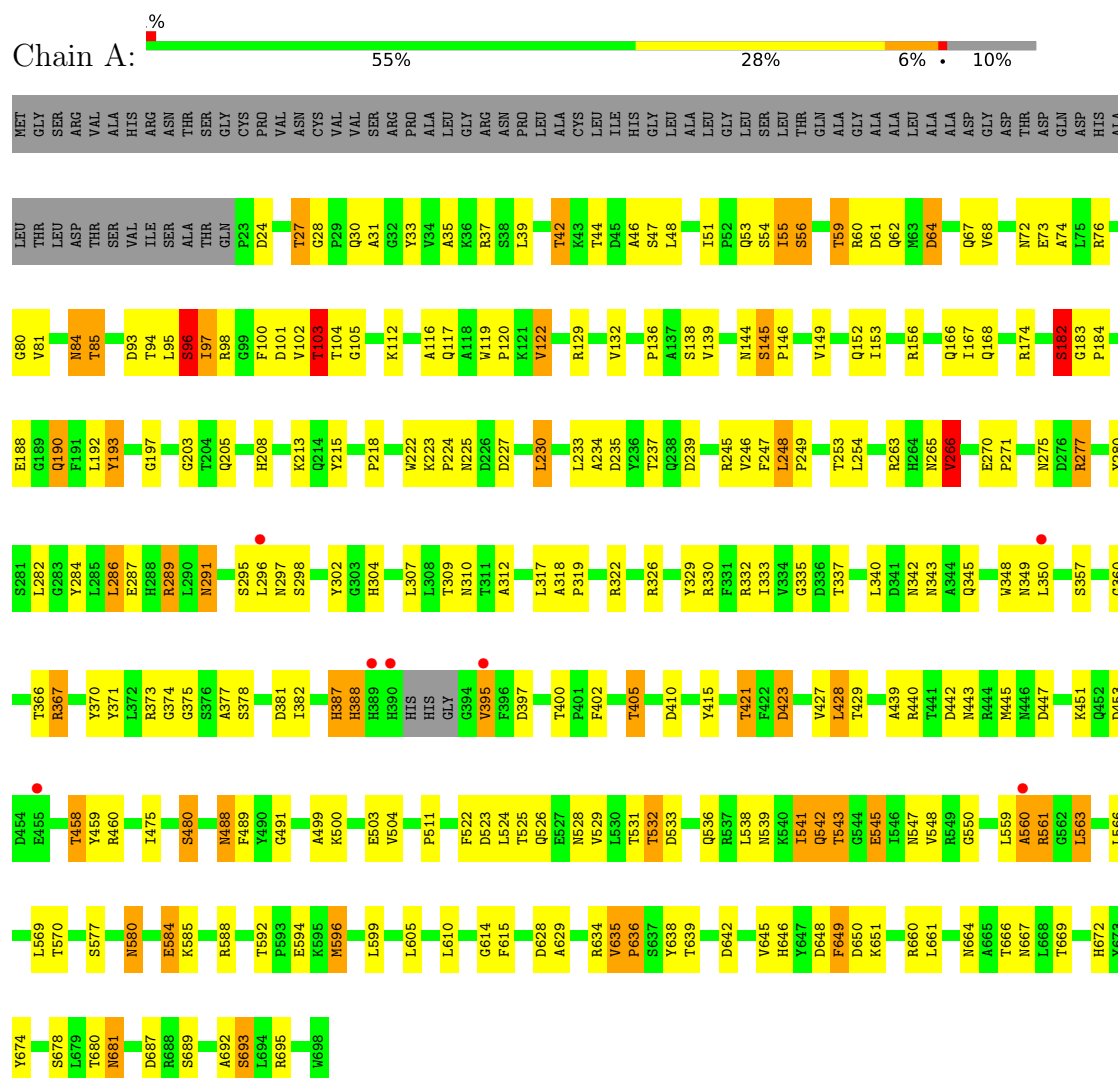


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	S	0	0
			22	14	1	2	3	2		
4	B	1	Total	C	Fe	N	O	S	0	0
			22	14	1	2	3	2		

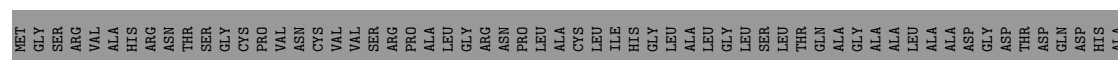
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Enantio-pyochelin receptor



• Molecule 1: Enantio-pyochelin receptor





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.07Å 170.83Å 232.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 3.26 48.57 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.57-3.26) 99.3 (48.57-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.259 0.214 , 0.256	Depositor DCC
R_{free} test set	2435 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	1.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10529	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: EFE, SO4, CIT

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	1.00	5/5350 (0.1%)	1.21	27/7273 (0.4%)
1	B	0.99	0/5328	1.22	24/7243 (0.3%)
All	All	0.99	5/10678 (0.0%)	1.22	51/14516 (0.4%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	THR	CA-CB	9.09	1.64	1.53
1	A	532	THR	CA-CB	6.91	1.62	1.53
1	A	395	VAL	CA-CB	6.34	1.61	1.54
1	A	97	ILE	CA-CB	-5.11	1.48	1.54
1	A	103	THR	CA-CB	5.03	1.62	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	PRO	CA-C-N	10.41	132.85	119.84
1	B	510	PRO	C-N-CA	10.41	132.85	119.84
1	B	270	GLU	CA-C-N	9.12	129.06	120.03
1	B	270	GLU	C-N-CA	9.12	129.06	120.03
1	A	266	VAL	CB-CA-C	-8.83	96.93	111.32
1	A	635	VAL	CA-C-N	8.64	130.64	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	VAL	C-N-CA	8.64	130.64	119.84
1	B	581	ASN	CA-C-N	8.24	130.15	119.84
1	B	581	ASN	C-N-CA	8.24	130.15	119.84
1	B	84	ASN	N-CA-C	8.07	123.31	113.38
1	A	681	ASN	N-CA-C	7.64	120.69	109.07
1	A	592	THR	CA-C-N	7.64	127.40	119.76
1	A	592	THR	C-N-CA	7.64	127.40	119.76
1	A	532	THR	CB-CA-C	7.53	122.63	110.29
1	B	28	GLY	CA-C-N	7.07	127.23	120.31
1	B	28	GLY	C-N-CA	7.07	127.23	120.31
1	A	442	ASP	N-CA-C	7.02	120.62	108.76
1	B	250	ALA	N-CA-C	-6.96	103.62	111.07
1	B	451	LYS	N-CA-C	-6.72	99.73	110.14
1	A	145	SER	CA-C-N	6.64	128.14	119.84
1	A	145	SER	C-N-CA	6.64	128.14	119.84
1	B	541	ILE	CB-CA-C	-6.41	100.96	110.82
1	A	84	ASN	N-CA-C	6.33	120.60	113.01
1	A	203	GLY	N-CA-C	-6.30	102.63	112.58
1	B	169	GLY	N-CA-C	-6.18	98.52	113.18
1	B	476	SER	N-CA-C	6.14	118.74	109.23
1	A	649	PHE	N-CA-C	5.92	117.42	110.97
1	A	596	MET	CB-CA-C	-5.86	103.44	110.94
1	A	439	ALA	N-CA-C	5.83	116.95	107.32
1	A	638	TYR	N-CA-C	5.82	117.25	108.46
1	B	635	VAL	CA-C-N	5.80	127.09	119.84
1	B	635	VAL	C-N-CA	5.80	127.09	119.84
1	B	34	VAL	N-CA-C	5.66	116.29	107.28
1	A	395	VAL	N-CA-C	5.64	116.07	108.17
1	B	203	GLY	N-CA-C	-5.59	104.92	112.57
1	B	103	THR	N-CA-C	-5.56	105.22	111.28
1	A	103	THR	N-CA-CB	5.33	119.24	110.39
1	B	144	ASN	N-CA-C	5.32	116.94	108.79
1	B	282	LEU	N-CA-C	-5.23	101.23	109.50
1	A	96	SER	N-CA-C	5.22	117.32	108.02
1	B	456	LYS	N-CA-C	5.22	117.01	108.76
1	A	116	ALA	N-CA-C	-5.20	105.69	111.36
1	B	334	VAL	N-CA-C	5.18	114.24	106.42
1	A	400	THR	CA-C-N	-5.17	114.39	119.92
1	A	400	THR	C-N-CA	-5.17	114.39	119.92
1	A	182	SER	N-CA-C	5.16	116.14	108.86
1	B	646	HIS	N-CA-C	5.14	116.74	108.32
1	A	190	GLN	N-CA-C	-5.13	106.86	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	GLY	N-CA-C	5.02	118.43	111.10
1	A	183	GLY	CA-C-N	5.00	124.90	119.85
1	A	183	GLY	C-N-CA	5.00	124.90	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	680	THR	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	5235	0	5045	160	0
1	B	5214	0	5026	168	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	13	0	5	5	0
3	B	13	0	5	6	0
4	A	22	0	11	4	0
4	B	22	0	11	0	0
All	All	10529	0	10103	335	0

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 16.

All (335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:HA	1:A:59:THR:HG21	1.29	1.09
1:B:317:LEU:HD11	1:B:382:ILE:HD11	1.32	1.09
1:A:680:THR:HG22	1:A:681:ASN:HD22	1.28	0.94
1:B:33:TYR:HA	1:B:59:THR:HG21	1.50	0.93
1:B:91:ARG:NH2	1:B:309:THR:HG21	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HH22	1:B:309:THR:CG2	1.82	0.93
1:A:248:LEU:O	1:A:681:ASN:HB2	1.71	0.91
1:B:91:ARG:HH22	1:B:309:THR:HG21	1.35	0.90
1:A:584:GLU:HG2	1:A:585:LYS:H	1.35	0.89
1:A:561:ARG:H	1:A:561:ARG:HD2	1.37	0.88
1:B:98:ARG:HG2	1:B:522:PHE:CZ	2.09	0.87
1:A:370:TYR:HB3	1:A:405:THR:HG22	1.55	0.86
1:A:30:GLN:HE22	1:A:35:ALA:HA	1.40	0.85
1:A:168:GLN:HB2	1:A:692:ALA:O	1.77	0.85
1:B:534:PRO:HD2	1:B:541:ILE:HD11	1.62	0.82
1:A:248:LEU:HD21	1:A:253:THR:HG21	1.62	0.81
3:A:700:CIT:O4	3:A:700:CIT:H22	1.80	0.80
1:B:424:GLU:O	1:B:425:HIS:HD2	1.63	0.80
1:A:614:GLY:HA3	1:A:646:HIS:CE1	2.15	0.80
1:A:545:GLU:OE2	1:A:580:ASN:HB2	1.82	0.78
1:B:71:VAL:HG13	1:B:130:ILE:HD13	1.64	0.77
3:A:700:CIT:H41	4:A:701:EFE:C18	2.16	0.76
1:A:680:THR:CG2	1:A:681:ASN:HD22	1.98	0.75
1:B:424:GLU:O	1:B:425:HIS:CD2	2.40	0.75
1:A:584:GLU:HG2	1:A:585:LYS:N	2.01	0.74
1:A:33:TYR:CA	1:A:59:THR:HG21	2.11	0.74
1:A:443:ASN:OD1	1:A:445:MET:HB2	1.88	0.73
1:A:421:THR:HG23	1:A:427:VAL:HG22	1.69	0.73
1:B:91:ARG:O	1:B:277:ARG:NH2	2.21	0.72
1:A:248:LEU:O	1:A:681:ASN:CB	2.38	0.72
1:A:310:ASN:HD21	1:A:330:ARG:HG3	1.55	0.72
1:A:560:ALA:HB3	1:A:561:ARG:HH11	1.56	0.71
1:B:237:THR:HB	1:B:279:GLN:HG3	1.71	0.71
1:A:561:ARG:H	1:A:561:ARG:CD	2.02	0.70
1:A:81:VAL:HG22	1:A:97:ILE:HG12	1.73	0.70
1:B:531:THR:HG21	1:B:580:ASN:H	1.56	0.70
1:B:560:ALA:HB3	1:B:561:ARG:NH1	2.06	0.70
1:A:531:THR:HG22	1:A:543:THR:HG22	1.71	0.70
1:A:375:GLY:HA3	1:A:397:ASP:O	1.94	0.68
1:B:68:VAL:HG12	1:B:73:GLU:HG2	1.75	0.68
1:B:123:GLU:OE1	1:B:213:LYS:HE2	1.94	0.68
1:B:138:SER:HB2	1:B:480:SER:HA	1.75	0.67
1:B:652:LEU:HD23	1:B:653:ILE:HG13	1.77	0.67
1:B:460:ARG:HB2	1:B:478:SER:HB3	1.77	0.66
1:B:168:GLN:HG3	1:B:176:GLN:HB3	1.76	0.66
1:B:471:LEU:HD23	1:B:508:TYR:HD1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HD12	1:A:102:VAL:HG11	1.78	0.66
1:B:471:LEU:HD23	1:B:508:TYR:CD1	2.32	0.65
1:B:91:ARG:NH2	1:B:309:THR:CG2	2.50	0.65
1:B:680:THR:HG22	1:B:681:ASN:HD22	1.62	0.65
1:A:122:VAL:HG21	1:A:152:GLN:OE1	1.96	0.65
1:B:168:GLN:HB3	1:B:693:SER:HB3	1.76	0.64
1:B:33:TYR:CA	1:B:59:THR:HG21	2.25	0.64
1:A:263:ARG:O	1:A:266:VAL:CG2	2.46	0.63
1:B:111:LEU:HD11	1:B:299:SER:HB2	1.81	0.63
1:B:317:LEU:HD23	1:B:321:LEU:HA	1.79	0.63
1:A:584:GLU:CG	1:A:585:LYS:N	2.61	0.63
1:B:631:ASN:N	1:B:631:ASN:HD22	1.97	0.63
1:B:63:MET:HE3	1:B:74:ALA:CB	2.29	0.62
1:A:193:TYR:CD1	1:A:193:TYR:C	2.75	0.62
1:A:680:THR:HG22	1:A:681:ASN:ND2	2.09	0.62
1:A:182:SER:C	1:A:193:TYR:HE1	2.07	0.62
1:A:184:PRO:HA	1:A:192:LEU:HD23	1.82	0.62
1:A:275:ASN:OD1	1:A:309:THR:HG23	2.00	0.62
1:A:531:THR:CG2	1:A:543:THR:HG22	2.30	0.62
1:B:343:ASN:C	1:B:343:ASN:HD22	2.08	0.62
1:B:350:LEU:O	1:B:351:GLY:O	2.18	0.61
1:B:306:ASN:HD22	1:B:334:VAL:HG22	1.66	0.61
1:B:245:ARG:HG2	3:B:700:CIT:H21	1.82	0.61
1:B:62:GLN:OE1	1:B:556:LYS:HE2	2.00	0.60
1:B:317:LEU:HD11	1:B:382:ILE:CD1	2.21	0.60
1:B:317:LEU:CD1	1:B:382:ILE:HD11	2.22	0.60
1:B:174:ARG:HA	1:B:202:SER:HB3	1.83	0.60
1:A:533:ASP:HB2	1:A:541:ILE:HG13	1.83	0.60
1:B:81:VAL:HG22	1:B:97:ILE:HG12	1.84	0.60
1:A:62:GLN:NE2	1:A:566:LEU:HD21	2.18	0.59
1:B:620:ARG:NH1	1:B:642:ASP:OD2	2.34	0.59
1:B:58:ILE:HD11	1:B:78:THR:OG1	2.03	0.58
1:A:68:VAL:HG21	1:A:74:ALA:HB2	1.83	0.58
1:B:104:THR:O	1:B:112:LYS:HE2	2.03	0.58
1:B:117:GLN:HB3	1:B:333:ILE:HD13	1.85	0.58
1:A:72:ASN:HB3	1:A:93:ASP:OD1	2.02	0.58
1:B:85:THR:HG22	1:B:94:THR:H	1.69	0.58
1:A:489:PHE:C	1:A:491:GLY:H	2.11	0.58
1:A:289:ARG:HD2	1:A:291:ASN:O	2.04	0.58
1:B:298:SER:HB2	1:B:342:ASN:ND2	2.19	0.58
1:A:168:GLN:OE1	1:A:174:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:GLN:NE2	1:A:538:LEU:HB2	2.19	0.57
1:A:208:HIS:CD2	1:A:271:PRO:HB3	2.39	0.57
1:A:310:ASN:ND2	1:A:330:ARG:HG3	2.20	0.57
1:A:98:ARG:O	1:A:100:PHE:HD1	1.87	0.56
1:A:122:VAL:HG21	1:A:152:GLN:CD	2.30	0.56
1:B:71:VAL:HG13	1:B:130:ILE:CD1	2.35	0.56
1:B:289:ARG:HG2	1:B:295:SER:HB3	1.87	0.56
1:A:117:GLN:HB3	1:A:333:ILE:HD13	1.88	0.56
1:B:168:GLN:OE1	1:B:174:ARG:NH1	2.38	0.56
1:B:270:GLU:OE2	1:B:387:HIS:HB3	2.05	0.56
1:B:560:ALA:HB3	1:B:561:ARG:HH12	1.69	0.56
1:B:68:VAL:HG11	1:B:74:ALA:HA	1.87	0.56
1:B:158:LEU:HD12	1:B:182:SER:HB3	1.88	0.56
1:A:280:TYR:CE1	1:A:304:HIS:HB3	2.41	0.56
1:B:355:MET:HE1	1:B:420:PHE:HE1	1.70	0.56
1:B:63:MET:HE3	1:B:74:ALA:HB1	1.88	0.56
1:B:343:ASN:C	1:B:343:ASN:ND2	2.65	0.55
1:A:428:LEU:HD12	1:A:429:THR:N	2.21	0.55
1:B:174:ARG:HA	1:B:202:SER:CB	2.36	0.55
1:B:198:LEU:HD23	1:B:198:LEU:C	2.32	0.55
1:B:647:TYR:OH	1:B:652:LEU:HB2	2.07	0.55
1:B:456:LYS:HG3	1:B:457:PHE:N	2.22	0.54
1:B:245:ARG:CG	3:B:700:CIT:H21	2.37	0.54
1:A:81:VAL:O	1:A:596:MET:HE1	2.07	0.54
1:A:138:SER:HB2	1:A:458:THR:HG21	1.90	0.54
1:A:213:LYS:HG3	1:A:239:ASP:HB3	1.89	0.54
1:B:340:LEU:HD12	1:B:341:ASP:H	1.73	0.54
1:A:263:ARG:O	1:A:266:VAL:HG22	2.08	0.54
1:B:79:ALA:HB2	1:B:568:ALA:HB1	1.90	0.54
1:B:207:ASP:O	1:B:267:PHE:CD2	2.61	0.54
1:B:503:GLU:HG3	1:B:522:PHE:HB3	1.90	0.54
1:A:193:TYR:O	1:A:193:TYR:HD1	1.92	0.53
1:A:488:ASN:CG	1:A:489:PHE:N	2.65	0.53
1:B:287:GLU:HG2	1:B:297:ASN:ND2	2.23	0.53
1:B:144:ASN:ND2	1:B:145:SER:O	2.42	0.53
1:B:291:ASN:HD21	1:B:294:TRP:HD1	1.56	0.53
1:A:129:ARG:HG3	1:A:153:ILE:HG13	1.91	0.53
1:A:222:TRP:CZ2	1:A:224:PRO:HG3	2.44	0.53
1:A:263:ARG:O	1:A:266:VAL:HG23	2.08	0.52
1:A:55:ILE:HG12	1:A:56:SER:N	2.24	0.52
1:A:101:ASP:OD2	1:A:103:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLN:HB3	1:A:693:SER:HB3	1.90	0.52
1:A:80:GLY:HA2	1:A:570:THR:HG21	1.91	0.52
1:B:281:SER:HB3	1:B:303:GLY:HA2	1.90	0.52
1:B:309:THR:HG23	1:B:331:PHE:CE1	2.45	0.52
1:B:222:TRP:CE2	1:B:224:PRO:HG3	2.46	0.51
1:B:88:ALA:HA	1:B:206:PHE:CE2	2.45	0.51
1:A:42:THR:HG21	1:A:46:ALA:CB	2.40	0.51
1:B:460:ARG:HG3	1:B:478:SER:HB3	1.93	0.51
1:A:253:THR:HB	1:A:674:TYR:CE1	2.45	0.51
1:B:530:LEU:HD12	1:B:530:LEU:H	1.76	0.51
1:B:245:ARG:HH11	3:B:700:CIT:H22	1.75	0.51
1:A:298:SER:OG	1:A:342:ASN:ND2	2.44	0.50
1:A:104:THR:O	1:A:112:LYS:NZ	2.44	0.50
1:A:423:ASP:CG	1:A:423:ASP:O	2.54	0.50
1:A:139:VAL:HG21	1:A:460:ARG:HB2	1.94	0.50
1:B:533:ASP:OD1	1:B:534:PRO:HD2	2.12	0.50
1:B:601:ALA:O	1:B:616:GLY:HA2	2.10	0.50
1:A:225:ASN:OD1	1:A:227:ASP:HB2	2.11	0.50
1:A:277:ARG:HB2	1:A:307:LEU:HA	1.93	0.50
1:B:225:ASN:C	1:B:227:ASP:H	2.20	0.50
1:B:680:THR:CG2	1:B:681:ASN:HD22	2.23	0.50
3:B:700:CIT:H22	3:B:700:CIT:O4	2.11	0.50
1:A:105:GLY:HA2	1:A:144:ASN:OD1	2.12	0.50
1:A:223:LYS:O	1:A:223:LYS:HG3	2.11	0.50
1:A:37:ARG:HB3	1:A:47:SER:HA	1.94	0.49
1:A:310:ASN:HD21	1:A:330:ARG:CG	2.23	0.49
1:B:245:ARG:CG	3:B:700:CIT:C2	2.90	0.49
1:A:332:ARG:HB3	1:A:371:TYR:CE2	2.46	0.49
1:A:218:PRO:HG2	1:A:234:ALA:HB3	1.93	0.49
1:B:285:LEU:HD23	1:B:299:SER:HB3	1.95	0.49
1:A:302:TYR:HA	1:A:337:THR:O	2.12	0.49
1:A:318:ALA:HB1	1:A:319:PRO:HD2	1.93	0.49
1:B:139:VAL:HG11	1:B:460:ARG:HB3	1.93	0.49
1:B:182:SER:CB	1:B:194:ARG:HG3	2.43	0.49
1:A:54:SER:HB2	1:A:503:GLU:OE2	2.12	0.49
1:A:193:TYR:CD1	1:A:193:TYR:O	2.66	0.49
1:A:559:LEU:HD12	1:A:563:LEU:HD23	1.95	0.49
1:B:182:SER:HB2	1:B:194:ARG:HG3	1.95	0.49
1:B:487:THR:HA	1:B:493:PRO:HA	1.93	0.49
1:A:298:SER:HA	1:A:342:ASN:HD22	1.78	0.49
1:B:348:TRP:N	1:B:348:TRP:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:ND2	1:A:345:GLN:NE2	2.60	0.49
1:A:666:THR:O	1:A:667:ASN:C	2.56	0.49
1:B:77:TYR:HA	1:B:598:SER:OG	2.13	0.49
1:A:421:THR:HG23	1:A:427:VAL:CG2	2.38	0.48
1:A:528:ASN:HA	1:A:542:GLN:O	2.13	0.48
1:A:536:GLN:HG3	1:A:539:ASN:HB2	1.94	0.48
1:B:200:ARG:NH1	1:B:211:ASP:CG	2.71	0.48
1:A:547:ASN:HD22	1:A:548:VAL:H	1.61	0.48
1:A:584:GLU:O	1:A:585:LYS:HB3	2.14	0.48
1:A:649:PHE:O	1:A:651:LYS:N	2.46	0.48
1:A:561:ARG:CD	1:A:561:ARG:N	2.76	0.48
1:B:434:GLN:NE2	1:B:457:PHE:HB2	2.28	0.48
1:A:59:THR:HG23	1:A:62:GLN:HB3	1.95	0.48
1:B:308:LEU:HG	1:B:309:THR:N	2.29	0.48
1:B:465:TYR:CD1	1:B:465:TYR:C	2.90	0.48
1:A:73:GLU:O	1:A:76:ARG:HG3	2.14	0.47
1:A:615:PHE:CD1	1:A:645:VAL:HG12	2.49	0.47
1:A:536:GLN:C	1:A:538:LEU:H	2.22	0.47
1:B:335:GLY:HA2	1:B:367:ARG:O	2.14	0.47
1:A:245:ARG:HG2	3:A:700:CIT:H21	1.95	0.47
1:A:67:GLN:HG3	1:A:664:ASN:OD1	2.14	0.47
1:B:85:THR:HG22	1:B:94:THR:N	2.29	0.47
1:B:322:ARG:HG2	1:B:381:ASP:OD1	2.14	0.47
1:B:420:PHE:CD2	1:B:428:LEU:HD23	2.50	0.47
1:B:545:GLU:HG3	1:B:577:SER:OG	2.14	0.47
1:B:300:ALA:HB2	1:B:340:LEU:HD13	1.97	0.47
1:B:128:GLU:HB2	1:B:155:LYS:HA	1.97	0.47
1:B:322:ARG:NH1	1:B:381:ASP:OD2	2.48	0.47
1:A:660:ARG:HD2	1:A:695:ARG:NH2	2.30	0.47
1:A:100:PHE:N	1:A:100:PHE:CD1	2.83	0.46
1:A:628:ASP:O	1:A:629:ALA:C	2.59	0.46
1:B:70:SER:HB2	1:B:72:ASN:ND2	2.31	0.46
1:B:270:GLU:HB3	1:B:273:LEU:HD11	1.97	0.46
1:B:284:TYR:CE2	1:B:300:ALA:HB3	2.50	0.46
1:B:245:ARG:HG2	3:B:700:CIT:C2	2.44	0.46
1:B:326:ARG:NH1	1:B:380:ILE:HG21	2.30	0.46
1:B:353:THR:HA	1:B:421:THR:O	2.15	0.46
1:B:288:HIS:CD2	1:B:288:HIS:C	2.94	0.46
1:B:318:ALA:HB1	1:B:319:PRO:CD	2.45	0.46
1:B:37:ARG:HD3	1:B:45:ASP:OD1	2.16	0.46
1:A:64:ASP:OD1	1:A:64:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:CE2	1:A:249:PRO:HG3	2.50	0.46
1:B:63:MET:CE	1:B:74:ALA:HB2	2.45	0.46
1:A:182:SER:HA	1:A:193:TYR:CE1	2.50	0.46
1:A:499:ALA:HA	1:A:525:THR:O	2.16	0.46
1:B:312:ALA:O	1:B:326:ARG:HD2	2.16	0.46
1:A:246:VAL:HG13	1:A:246:VAL:O	2.16	0.45
1:A:284:TYR:CD1	1:A:284:TYR:C	2.94	0.45
1:A:526:GLN:HG2	1:A:529:VAL:HG22	1.98	0.45
1:B:298:SER:CB	1:B:342:ASN:ND2	2.80	0.45
1:A:30:GLN:NE2	1:A:35:ALA:HA	2.19	0.45
1:B:57:VAL:HG22	1:B:131:ASP:OD1	2.15	0.45
1:A:348:TRP:H	1:A:348:TRP:CD1	2.34	0.45
1:A:522:PHE:CD1	1:A:522:PHE:C	2.94	0.45
1:A:528:ASN:O	1:A:542:GLN:NE2	2.50	0.45
1:B:420:PHE:HB2	1:B:428:LEU:HB3	1.99	0.45
1:B:591:ASP:HA	1:B:625:THR:OG1	2.16	0.45
1:A:136:PRO:HB3	1:A:480:SER:HB3	1.97	0.45
1:A:642:ASP:OD1	1:A:666:THR:HA	2.16	0.45
1:A:547:ASN:HD22	1:A:548:VAL:N	2.14	0.45
1:B:501:GLN:HG3	1:B:524:LEU:HD13	1.99	0.45
1:A:72:ASN:CG	1:A:85:THR:HG23	2.41	0.45
1:A:197:GLY:HA2	1:A:215:TYR:O	2.16	0.45
1:B:55:ILE:HG23	1:B:55:ILE:O	2.16	0.45
1:B:201:ASP:HA	1:B:212:ASP:OD1	2.15	0.45
1:B:168:GLN:CB	1:B:692:ALA:O	2.65	0.45
1:B:60:ARG:HA	1:B:60:ARG:HD2	1.84	0.45
1:A:205:GLN:HG3	1:A:265:ASN:ND2	2.32	0.44
1:B:63:MET:CE	1:B:74:ALA:CB	2.96	0.44
1:B:267:PHE:CD1	1:B:267:PHE:C	2.96	0.44
1:B:605:LEU:HA	1:B:606:PRO:HD3	1.84	0.44
1:A:488:ASN:CG	1:A:489:PHE:H	2.24	0.44
3:A:700:CIT:C4	4:A:701:EFE:C18	2.90	0.44
1:A:348:TRP:CD1	1:A:348:TRP:N	2.84	0.44
1:A:374:GLY:HA3	1:A:402:PHE:CE1	2.52	0.44
1:A:459:TYR:N	1:A:459:TYR:CD1	2.85	0.44
1:A:503:GLU:HG3	1:A:522:PHE:HB3	1.99	0.44
1:B:477:TYR:HA	1:B:501:GLN:O	2.17	0.44
1:A:230:LEU:HB2	1:A:286:LEU:HD12	1.98	0.44
1:B:317:LEU:HD23	1:B:321:LEU:HD22	2.00	0.44
1:A:222:TRP:CE2	1:A:224:PRO:HG3	2.53	0.44
1:B:306:ASN:ND2	1:B:334:VAL:HG22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:HB3	1:A:190:GLN:HG3	2.00	0.44
1:B:668:LEU:HA	1:B:688:ARG:HG3	1.99	0.44
1:B:265:ASN:N	1:B:265:ASN:HD22	2.15	0.44
1:B:631:ASN:N	1:B:631:ASN:ND2	2.65	0.44
1:A:270:GLU:OE1	1:A:387:HIS:HB3	2.18	0.43
1:A:31:ALA:HA	1:A:61:ASP:OD2	2.18	0.43
1:B:51:ILE:HA	1:B:52:PRO:HD3	1.81	0.43
1:B:355:MET:HE1	1:B:420:PHE:CE1	2.53	0.43
1:A:254:LEU:HD22	1:A:635:VAL:HG22	2.00	0.43
1:B:159:ASP:OD1	1:B:159:ASP:N	2.51	0.43
1:B:198:LEU:HD23	1:B:199:GLU:N	2.32	0.43
1:A:119:TRP:HA	1:A:120:PRO:HD3	1.79	0.43
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.78	0.43
1:A:360:GLY:HA3	1:A:415:TYR:CZ	2.53	0.43
1:B:532:THR:CG2	1:B:581:ASN:HB2	2.48	0.43
4:A:701:EFE:H14	4:A:701:EFE:C19	2.49	0.43
1:A:523:ASP:C	1:A:523:ASP:OD1	2.61	0.43
1:B:91:ARG:H	1:B:91:ARG:HG3	1.59	0.43
1:A:312:ALA:O	1:A:326:ARG:HD2	2.18	0.43
1:A:335:GLY:HA2	1:A:367:ARG:O	2.19	0.43
1:B:140:LEU:O	1:B:433:ARG:NH1	2.51	0.43
1:B:213:LYS:HG3	1:B:239:ASP:HB3	2.01	0.43
1:A:84:ASN:ND2	1:A:96:SER:HB2	2.34	0.43
1:B:142:GLY:O	1:B:143:GLN:C	2.61	0.42
1:B:464:VAL:HG12	1:B:465:TYR:N	2.33	0.42
1:A:388:HIS:CD2	1:A:388:HIS:N	2.87	0.42
1:B:62:GLN:O	1:B:66:GLN:HG3	2.18	0.42
1:A:136:PRO:HD3	1:A:524:LEU:HD13	2.01	0.42
1:A:42:THR:HG21	1:A:46:ALA:HB2	2.01	0.42
1:A:317:LEU:HA	1:A:317:LEU:HD12	1.84	0.42
1:B:201:ASP:OD1	1:B:201:ASP:C	2.62	0.42
1:B:226:ASP:OD1	1:B:226:ASP:N	2.49	0.42
1:A:168:GLN:HE21	1:A:693:SER:HB3	1.84	0.42
1:B:155:LYS:HD3	1:B:194:ARG:NH1	2.34	0.42
1:A:145:SER:HA	1:A:146:PRO:HD2	1.68	0.42
1:A:297:ASN:HD22	1:A:345:GLN:NE2	2.17	0.42
1:B:619:VAL:HG22	1:B:641:LEU:CD2	2.49	0.42
1:B:340:LEU:HD12	1:B:341:ASP:N	2.34	0.42
1:B:160:LYS:HA	1:B:161:PRO:HD3	1.90	0.42
1:B:553:LEU:HD12	1:B:554:GLU:N	2.35	0.42
1:A:27:THR:HG21	1:A:156:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HD23	1:A:559:LEU:HA	1.80	0.42
1:B:263:ARG:HH21	1:B:265:ASN:HB2	1.84	0.42
1:A:27:THR:HG22	1:A:28:GLY:N	2.34	0.41
1:A:322:ARG:NH1	1:A:381:ASP:OD2	2.53	0.41
1:A:348:TRP:HZ3	1:A:350:LEU:HB2	1.85	0.41
1:B:24:ASP:OD2	1:B:36:LYS:HE2	2.20	0.41
1:A:672:HIS:ND1	1:A:687:ASP:OD1	2.53	0.41
1:B:136:PRO:HG2	1:B:501:GLN:HB2	2.02	0.41
1:B:659:LEU:HD12	1:B:695:ARG:O	2.20	0.41
1:A:445:MET:HE2	1:A:445:MET:HA	2.00	0.41
1:B:275:ASN:OD1	1:B:309:THR:HB	2.20	0.41
1:B:649:PHE:O	1:B:650:ASP:C	2.63	0.41
1:A:105:GLY:O	1:A:149:VAL:HA	2.21	0.41
1:B:404:ASN:HB2	1:B:445:MET:HE3	2.02	0.41
4:A:701:EFE:C19	4:A:701:EFE:C14	2.99	0.41
1:B:626:GLU:OE1	1:B:631:ASN:HA	2.21	0.41
1:A:329:TYR:HA	1:A:373:ARG:O	2.21	0.41
1:B:299:SER:O	1:B:340:LEU:HD12	2.21	0.41
1:B:510:PRO:HA	1:B:511:PRO:HD2	1.72	0.41
1:A:122:VAL:CG2	1:A:152:GLN:OE1	2.65	0.41
1:A:377:ALA:O	1:A:378:SER:C	2.61	0.41
1:B:460:ARG:CB	1:B:478:SER:HB3	2.46	0.41
1:B:621:TYR:CD1	1:B:621:TYR:C	2.99	0.41
1:A:42:THR:HG23	1:A:44:THR:O	2.21	0.41
1:A:547:ASN:ND2	1:A:548:VAL:N	2.69	0.41
1:B:350:LEU:HB3	1:B:351:GLY:H	1.66	0.41
1:B:108:ARG:HA	1:B:152:GLN:O	2.21	0.40
1:B:350:LEU:HD12	1:B:350:LEU:HA	1.82	0.40
1:A:635:VAL:HA	1:A:636:PRO:HD2	1.74	0.40
1:A:646:HIS:HA	1:A:661:LEU:O	2.21	0.40
1:B:462:GLY:HA2	1:B:475:ILE:O	2.21	0.40
1:A:440:ARG:HG2	1:A:451:LYS:HG3	2.02	0.40
1:B:527:GLU:O	1:B:528:ASN:HB2	2.21	0.40
1:B:666:THR:O	1:B:667:ASN:C	2.63	0.40
1:A:97:ILE:O	1:A:98:ARG:C	2.63	0.40
1:A:280:TYR:CE1	1:A:304:HIS:CB	3.05	0.40
3:A:700:CIT:O4	3:A:700:CIT:C2	2.62	0.40
1:B:364:ARG:HB2	1:B:411:GLN:HB2	2.02	0.40
1:A:98:ARG:O	1:A:100:PHE:CD1	2.71	0.40
1:B:136:PRO:HB3	1:B:480:SER:HB3	2.02	0.40
1:B:182:SER:OG	1:B:194:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:TRP:HE3	1:B:463:LEU:HD11	1.87	0.40
1:B:460:ARG:CG	1:B:478:SER:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	669/748 (89%)	598 (89%)	62 (9%)	9 (1%)	9	34
1	B	666/748 (89%)	603 (90%)	47 (7%)	16 (2%)	4	23
All	All	1335/1496 (89%)	1201 (90%)	109 (8%)	25 (2%)	6	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	560	ALA
1	A	650	ASP
1	B	351	GLY
1	B	511	PRO
1	B	560	ALA
1	B	591	ASP
1	B	650	ASP
1	A	42	THR
1	A	291	ASN
1	A	488	ASN
1	B	139	VAL
1	B	532	THR
1	B	537	ARG
1	B	629	ALA
1	A	636	PRO
1	B	425	HIS

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Mol	Chain	Res	Type
1	A	235	ASP
1	B	161	PRO
1	B	113	GLY
1	B	398	PRO
1	B	606	PRO
1	A	580	ASN
1	B	561	ARG
1	B	609	PRO
1	A	511	PRO

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	561/618 (91%)	485 (86%)	76 (14%)	4	16
1	B	559/618 (90%)	466 (83%)	93 (17%)	2	10
All	All	1120/1236 (91%)	951 (85%)	169 (15%)	3	13

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	27	THR
1	A	39	LEU
1	A	48	LEU
1	A	51	ILE
1	A	53	GLN
1	A	55	ILE
1	A	56	SER
1	A	59	THR
1	A	60	ARG
1	A	64	ASP
1	A	85	THR
1	A	95	LEU
1	A	96	SER

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Mol	Chain	Res	Type
1	A	103	THR
1	A	122	VAL
1	A	132	VAL
1	A	166	GLN
1	A	167	ILE
1	A	182	SER
1	A	193	TYR
1	A	230	LEU
1	A	237	THR
1	A	248	LEU
1	A	266	VAL
1	A	277	ARG
1	A	282	LEU
1	A	286	LEU
1	A	287	GLU
1	A	289	ARG
1	A	295	SER
1	A	296	LEU
1	A	340	LEU
1	A	343	ASN
1	A	349	ASN
1	A	357	SER
1	A	366	THR
1	A	367	ARG
1	A	382	ILE
1	A	387	HIS
1	A	388	HIS
1	A	395	VAL
1	A	405	THR
1	A	410	ASP
1	A	421	THR
1	A	423	ASP
1	A	428	LEU
1	A	447	ASP
1	A	453	ASP
1	A	458	THR
1	A	475	ILE
1	A	480	SER
1	A	500	LYS
1	A	504	VAL
1	A	532	THR
1	A	541	ILE

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Mol	Chain	Res	Type
1	A	542	GLN
1	A	543	THR
1	A	545	GLU
1	A	561	ARG
1	A	563	LEU
1	A	569	LEU
1	A	577	SER
1	A	584	GLU
1	A	588	ARG
1	A	594	GLU
1	A	599	LEU
1	A	605	LEU
1	A	610	LEU
1	A	634	ARG
1	A	639	THR
1	A	648	ASP
1	A	669	THR
1	A	678	SER
1	A	689	SER
1	A	693	SER
1	B	24	ASP
1	B	27	THR
1	B	47	SER
1	B	54	SER
1	B	55	ILE
1	B	59	THR
1	B	72	ASN
1	B	85	THR
1	B	94	THR
1	B	95	LEU
1	B	98	ARG
1	B	103	THR
1	B	104	THR
1	B	108	ARG
1	B	122	VAL
1	B	136	PRO
1	B	158	LEU
1	B	159	ASP
1	B	160	LYS
1	B	165	VAL
1	B	182	SER
1	B	185	LEU

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Mol	Chain	Res	Type
1	B	187	ASP
1	B	190	GLN
1	B	201	ASP
1	B	223	LYS
1	B	225	ASN
1	B	226	ASP
1	B	263	ARG
1	B	265	ASN
1	B	278	THR
1	B	288	HIS
1	B	293	VAL
1	B	295	SER
1	B	296	LEU
1	B	299	SER
1	B	305	VAL
1	B	309	THR
1	B	317	LEU
1	B	321	LEU
1	B	343	ASN
1	B	348	TRP
1	B	349	ASN
1	B	350	LEU
1	B	352	SER
1	B	354	GLN
1	B	356	VAL
1	B	359	LEU
1	B	376	SER
1	B	384	ASN
1	B	386	VAL
1	B	387	HIS
1	B	400	THR
1	B	405	THR
1	B	408	ARG
1	B	414	VAL
1	B	424	GLU
1	B	453	ASP
1	B	458	THR
1	B	460	ARG
1	B	461	THR
1	B	475	ILE
1	B	480	SER
1	B	492	THR

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Mol	Chain	Res	Type
1	B	498	SER
1	B	501	GLN
1	B	506	VAL
1	B	517	ILE
1	B	518	THR
1	B	526	GLN
1	B	530	LEU
1	B	531	THR
1	B	541	ILE
1	B	561	ARG
1	B	563	LEU
1	B	565	LEU
1	B	566	LEU
1	B	569	LEU
1	B	570	THR
1	B	578	LYS
1	B	583	LEU
1	B	592	THR
1	B	625	THR
1	B	631	ASN
1	B	636	PRO
1	B	637	SER
1	B	645	VAL
1	B	652	LEU
1	B	666	THR
1	B	668	LEU
1	B	681	ASN
1	B	689	SER
1	B	691	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	69	GLN
1	A	114	ASN
1	A	117	GLN
1	A	163	HIS
1	A	166	GLN
1	A	208	HIS
1	A	238	GLN
1	A	259	ASN

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Mol	Chain	Res	Type
1	A	297	ASN
1	A	342	ASN
1	A	345	GLN
1	A	384	ASN
1	A	407	GLN
1	A	417	GLN
1	A	418	GLN
1	A	434	GLN
1	A	469	ASN
1	A	542	GLN
1	A	547	ASN
1	A	572	ASN
1	A	681	ASN
1	B	72	ASN
1	B	82	GLN
1	B	84	ASN
1	B	190	GLN
1	B	259	ASN
1	B	297	ASN
1	B	306	ASN
1	B	342	ASN
1	B	343	ASN
1	B	345	GLN
1	B	349	ASN
1	B	387	HIS
1	B	388	HIS
1	B	407	GLN
1	B	411	GLN
1	B	418	GLN
1	B	425	HIS
1	B	434	GLN
1	B	681	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	CIT	B	700	4	12,12,12	2.64	3 (25%)	17,17,17	1.88	4 (23%)
4	EFE	A	701	3	20,27,27	2.66	5 (25%)	24,46,46	3.18	11 (45%)
2	SO4	B	699	-	4,4,4	0.20	0	6,6,6	0.29	0
2	SO4	A	699	-	4,4,4	0.25	0	6,6,6	0.24	0
3	CIT	A	700	4	12,12,12	2.60	3 (25%)	17,17,17	2.28	7 (41%)
4	EFE	B	701	3	20,27,27	2.54	6 (30%)	24,46,46	3.29	9 (37%)

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
4	EFE	B	701	3	-	-	0/6/6/6
3	CIT	A	700	4	-	9/16/16/16	-
3	CIT	B	700	4	-	11/16/16/16	-
4	EFE	A	701	3	1/1/8/8	-	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	EFE	C14-N1	-9.23	1.42	1.50
3	B	700	CIT	O4-C5	7.38	1.55	1.30
4	B	701	EFE	C14-N1	-6.79	1.44	1.50
3	A	700	CIT	O4-C5	6.07	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	CIT	O2-C1	5.65	1.49	1.30
4	A	701	EFE	O20-C19	4.96	1.33	1.21
4	B	701	EFE	O20-C19	4.81	1.33	1.21
4	B	701	EFE	O1-C1	4.70	1.38	1.32
3	B	700	CIT	O2-C1	4.52	1.45	1.30
4	B	701	EFE	C15-N2	-4.10	1.45	1.50
4	A	701	EFE	C15-N2	-3.72	1.46	1.50
4	B	701	EFE	C17-C19	-3.05	1.46	1.53
4	A	701	EFE	C17-C19	-2.72	1.47	1.53
4	B	701	EFE	C12-S1	2.59	1.79	1.74
4	A	701	EFE	O1-C1	2.51	1.35	1.32
3	A	700	CIT	O5-C6	2.15	1.28	1.22
3	B	700	CIT	O5-C6	2.04	1.28	1.22

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	EFE	C14-C15-N2	-10.85	97.37	110.74
4	B	701	EFE	C14-C15-N2	-10.72	97.52	110.74
4	A	701	EFE	C15-C14-N1	-6.59	100.09	107.34
4	B	701	EFE	C18-N2-C17	5.85	111.95	107.54
4	B	701	EFE	C15-C14-N1	-5.64	101.13	107.34
3	B	700	CIT	O3-C5-C4	-4.73	109.56	122.95
3	A	700	CIT	C2-C3-C6	4.64	120.29	110.03
3	A	700	CIT	O2-C1-C2	3.79	126.34	114.35
4	B	701	EFE	C15-N2-C17	3.61	111.49	101.91
4	B	701	EFE	S1-C12-N1	-3.44	113.48	118.50
4	B	701	EFE	C16-C17-C19	-3.42	104.25	112.56
3	B	700	CIT	O4-C5-C4	3.41	125.15	114.35
3	A	700	CIT	O6-C6-C3	3.33	119.53	113.14
4	A	701	EFE	C15-N2-C17	3.32	110.72	101.91
4	A	701	EFE	O21-C19-C17	-3.27	112.28	116.35
4	B	701	EFE	O21-C19-C17	-3.11	112.48	116.35
4	A	701	EFE	C18-N2-C17	3.10	109.87	107.54
3	B	700	CIT	O7-C3-C6	-3.02	104.68	108.96
4	A	701	EFE	C1-C6-C12	2.93	126.10	120.98
4	A	701	EFE	S1-C12-N1	-2.80	114.42	118.50
4	A	701	EFE	C16-C17-C19	-2.80	105.75	112.56
3	B	700	CIT	O6-C6-C3	2.73	118.38	113.14
3	A	700	CIT	C4-C3-C6	-2.69	104.09	110.03
3	A	700	CIT	O1-C1-C2	-2.65	115.45	122.95
4	A	701	EFE	C13-S1-C12	2.57	92.20	89.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	EFE	C13-S1-C12	2.50	92.12	89.59
3	A	700	CIT	O7-C3-C2	-2.42	103.86	109.38
4	B	701	EFE	C1-C6-C12	2.36	125.11	120.98
4	A	701	EFE	C5-C6-C12	-2.33	115.40	119.48
4	A	701	EFE	O20-C19-C17	2.13	123.35	119.19
3	A	700	CIT	O2-C1-O1	-2.00	118.18	123.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	701	EFE	N1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	CIT	O7-C3-C6-O5
3	A	700	CIT	O7-C3-C6-O6
3	A	700	CIT	C4-C3-C6-O5
3	A	700	CIT	C4-C3-C6-O6
3	B	700	CIT	C1-C2-C3-O7
3	B	700	CIT	C1-C2-C3-C6
3	B	700	CIT	C2-C3-C6-O5
3	B	700	CIT	C2-C3-C6-O6
3	B	700	CIT	O7-C3-C6-O5
3	B	700	CIT	O7-C3-C6-O6
3	B	700	CIT	C1-C2-C3-C4
3	B	700	CIT	C4-C3-C6-O5
3	A	700	CIT	C1-C2-C3-C4
3	A	700	CIT	C1-C2-C3-C6
3	A	700	CIT	O7-C3-C4-C5
3	B	700	CIT	C4-C3-C6-O6
3	A	700	CIT	C6-C3-C4-C5
3	A	700	CIT	C2-C3-C4-C5
3	B	700	CIT	C3-C4-C5-O4
3	B	700	CIT	C3-C4-C5-O3

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	CIT	6	0

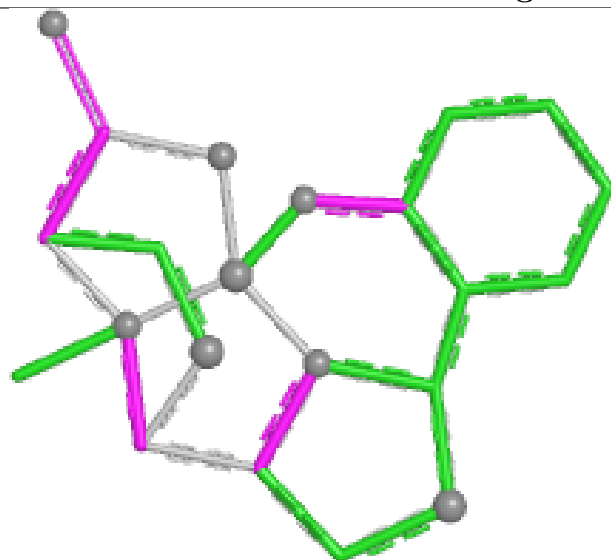
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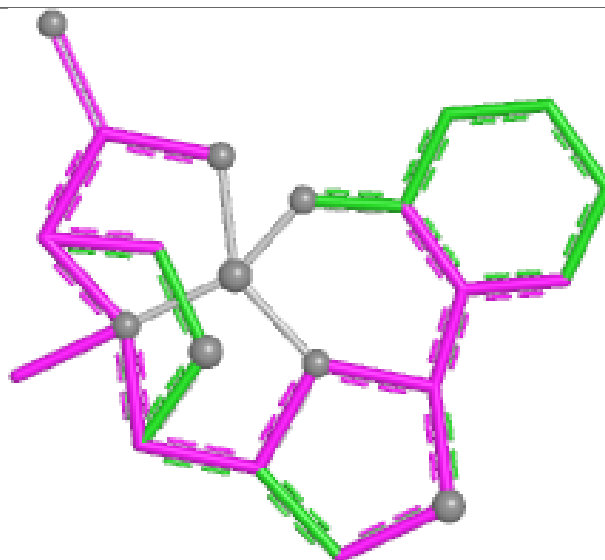
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	EFE	4	0
3	A	700	CIT	5	0

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 than 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.

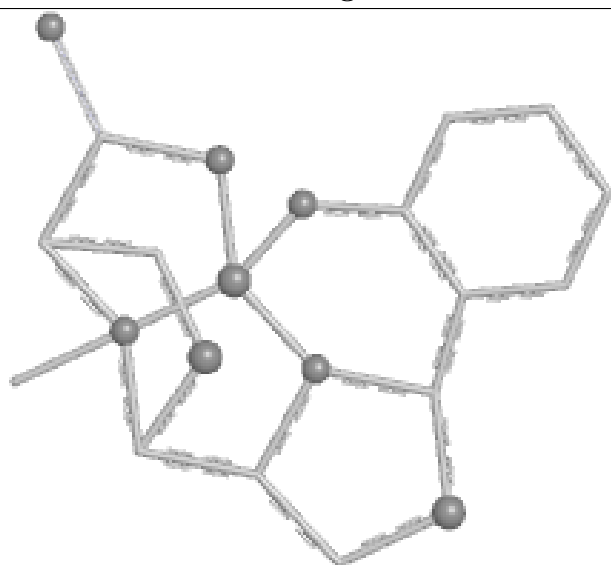
Ligand EFE A 701



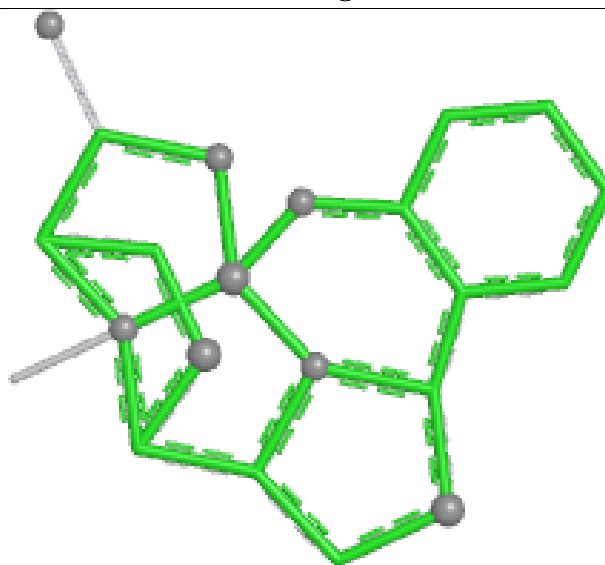
Bond lengths



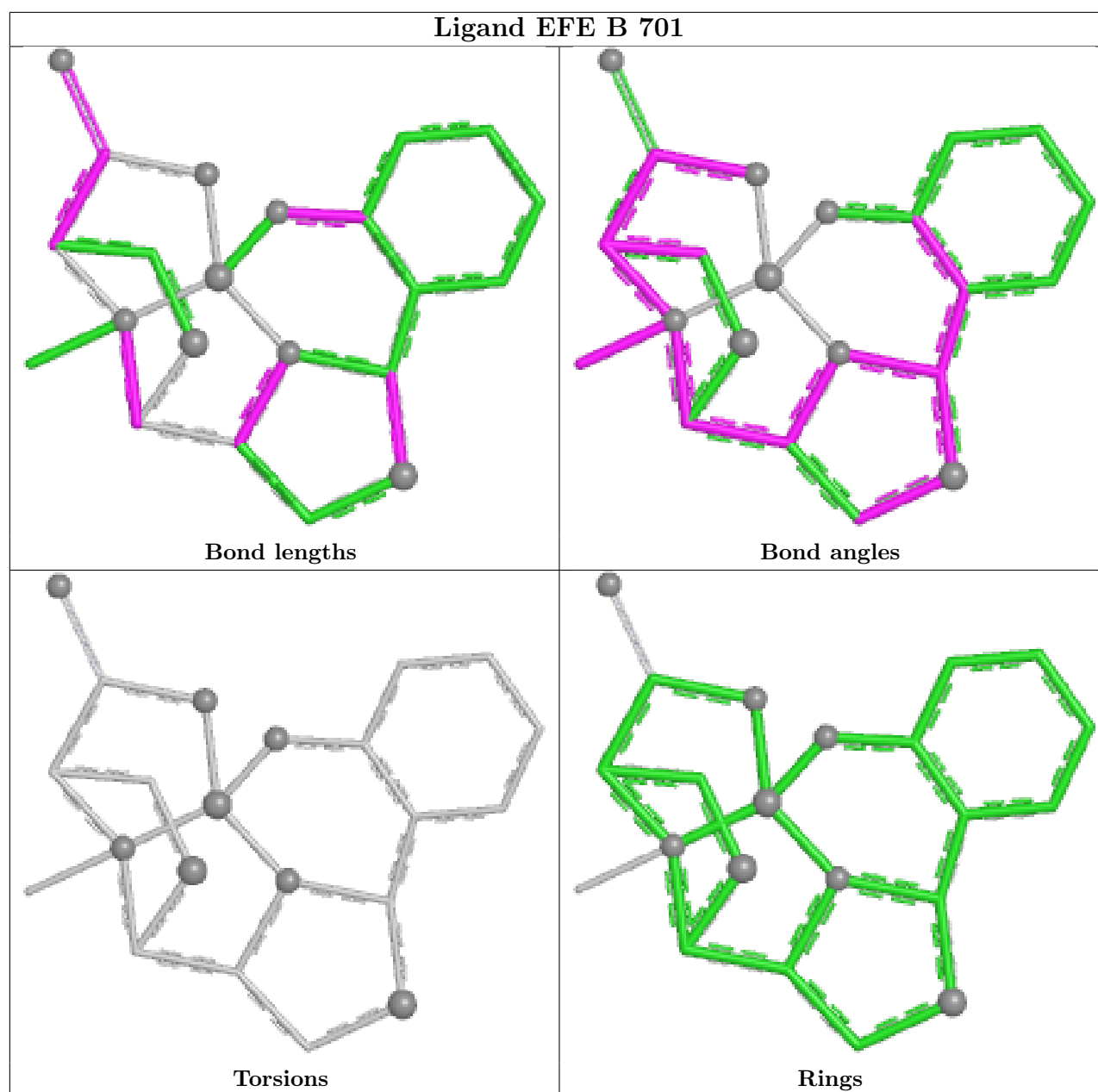
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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	A	673/748 (89%)	-0.01	7 (1%)	79 62	48, 68, 98, 118	0
1	B	670/748 (89%)	-0.09	2 (0%)	90 82	46, 67, 93, 116	0
All	All	1343/1496 (89%)	-0.05	9 (0%)	84 70	46, 68, 95, 118	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	HIS	5.9
1	A	350	LEU	5.1
1	A	296	LEU	4.0
1	A	389	HIS	3.6
1	B	395	VAL	3.1
1	A	395	VAL	2.4
1	B	388	HIS	2.3
1	A	560	ALA	2.3
1	A	455	GLU	2.1

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 oligosaccharides 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,

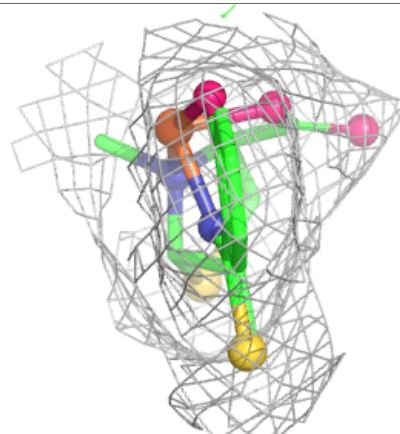
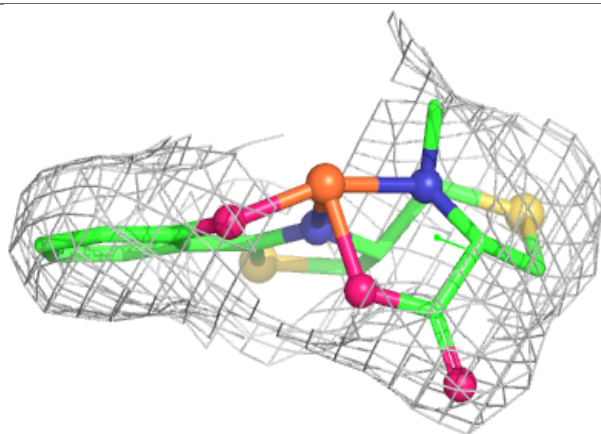
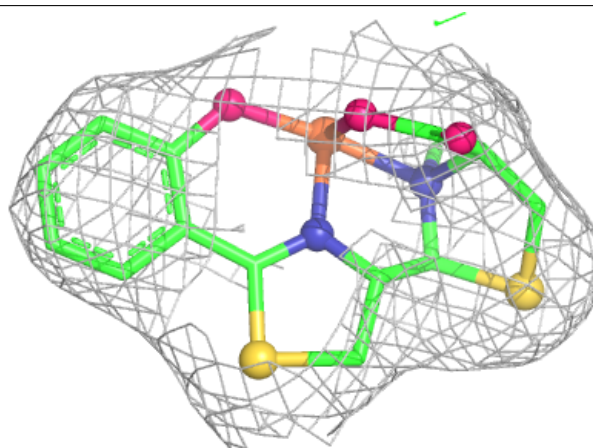
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIT	B	700	13/13	0.75	0.14	73,81,90,90	0
3	CIT	A	700	13/13	0.81	0.14	66,76,87,87	0
2	SO4	B	699	5/5	0.91	0.10	96,97,98,98	0
2	SO4	A	699	5/5	0.97	0.08	97,97,98,98	0
4	EFE	A	701	22/22	0.99	0.05	59,62,64,65	0
4	EFE	B	701	22/22	0.99	0.06	67,68,70,71	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.

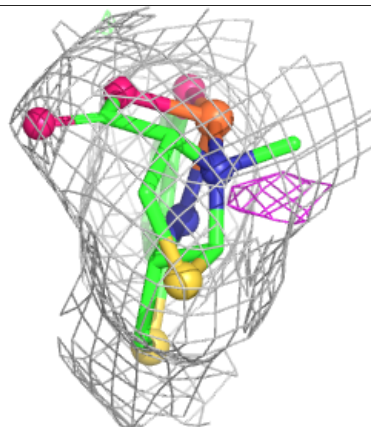
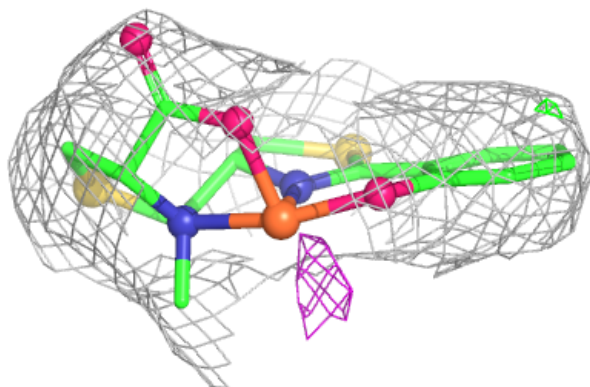
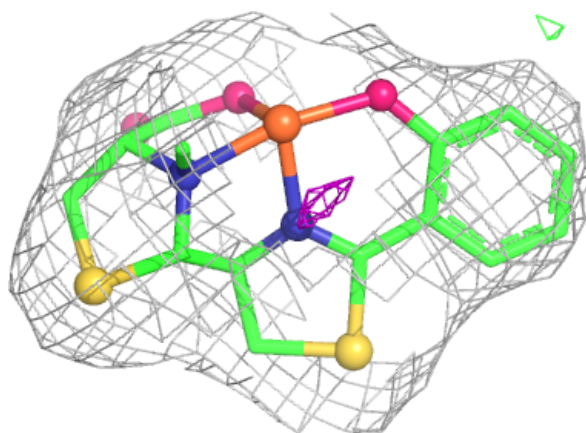
Electron density around EFE A 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EFE B 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.