Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2022 – 01:09 pm BST

PDB ID	:	7ZFA
Title	:	SARS-CoV-2 Omicron RBD in complex with Omi-6 and COVOX-150 Fabs
Authors	:	Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.
Deposited on	:	2022-04-01
Resolution	:	4.24 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 following versions of software and data (see references ⓘ) were used in the production of this report:

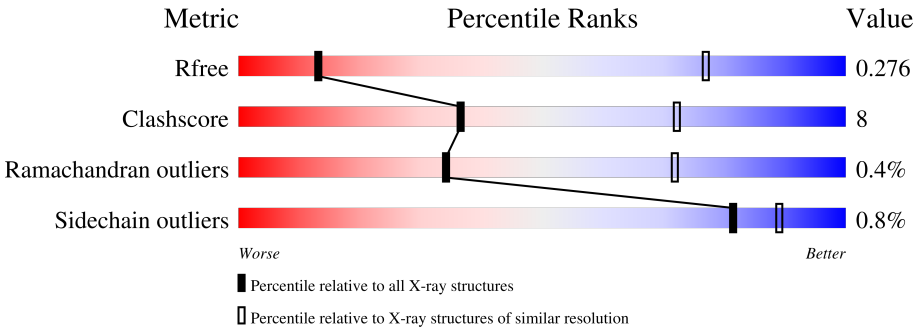
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.24 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}	130704	1015 (4.70-3.78)
Clashscore	141614	1051 (4.68-3.80)
Ramachandran outliers	138981	1007 (4.68-3.80)
Sidechain outliers	138945	1016 (4.70-3.78)

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%

Mol	Chain	Length	Quality of chain
1	A	202	82% 14% ·
1	B	202	82% 13% ·
1	C	202	80% 16% ·
1	D	202	82% 14% ·
2	E	229	85% 13% ·
2	H	229	83% 14% · ·
2	J	229	82% 15% · ·

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Mol	Chain	Length	Quality of chain
2	M	229	86% 11%
3	F	214	86% 13%
3	K	214	86% 12%
3	L	214	86% 13%
3	N	214	91% 7%
4	O	222	85% 11%
4	Q	222	82% 14%
4	S	222	86% 11%
4	X	222	85% 12%
5	P	216	86% 13%
5	R	216	89% 9%
5	T	216	87% 12%
5	Y	216	90% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31966 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	195	Total	C	N	O	S	0	0	0
			1557	1001	264	284	8			
1	B	194	Total	C	N	O	S	0	0	0
			1550	997	263	282	8			
1	C	195	Total	C	N	O	S	0	0	0
			1551	998	262	283	8			
1	A	195	Total	C	N	O	S	0	0	0
			1556	1001	264	283	8			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	327	HIS	-	expression tag	UNP P0DTC2
D	328	HIS	-	expression tag	UNP P0DTC2
D	329	HIS	-	expression tag	UNP P0DTC2
D	330	HIS	-	expression tag	UNP P0DTC2
D	331	HIS	-	expression tag	UNP P0DTC2
D	332	HIS	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	371	LEU	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	493	ARG	GLN	variant	UNP P0DTC2
D	496	SER	GLY	variant	UNP P0DTC2
D	498	ARG	GLN	conflict	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	527	LYS	-	expression tag	UNP P0DTC2
D	528	LYS	-	expression tag	UNP P0DTC2
B	327	HIS	-	expression tag	UNP P0DTC2
B	328	HIS	-	expression tag	UNP P0DTC2
B	329	HIS	-	expression tag	UNP P0DTC2
B	330	HIS	-	expression tag	UNP P0DTC2
B	331	HIS	-	expression tag	UNP P0DTC2
B	332	HIS	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	527	LYS	-	expression tag	UNP P0DTC2
B	528	LYS	-	expression tag	UNP P0DTC2
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	527	LYS	-	expression tag	UNP P0DTC2
C	528	LYS	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Omi-6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1605	1006	269	323	7			
2	M	224	Total	C	N	O	S	0	0	0
			1615	1015	270	323	7			
2	J	224	Total	C	N	O	S	0	0	0
			1608	1010	269	322	7			
2	H	224	Total	C	N	O	S	0	0	0
			1615	1015	270	323	7			

- Molecule 3 is a protein called Omi-6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	212	Total	C	N	O	S	0	0	0
			1603	998	273	327	5			
3	K	211	Total	C	N	O	S	0	0	0
			1592	994	268	325	5			
3	N	210	Total	C	N	O	S	0	0	0
			1581	986	267	323	5			
3	L	211	Total	C	N	O	S	0	0	0
			1604	1002	272	325	5			

- Molecule 4 is a protein called COVOX-150 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			
4	S	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			
4	O	214	Total	C	N	O	S	0	0	0
			1583	997	263	314	9			
4	Q	215	Total	C	N	O	S	0	0	0
			1592	1002	265	316	9			

- Molecule 5 is a protein called COVOX-150 light chain.

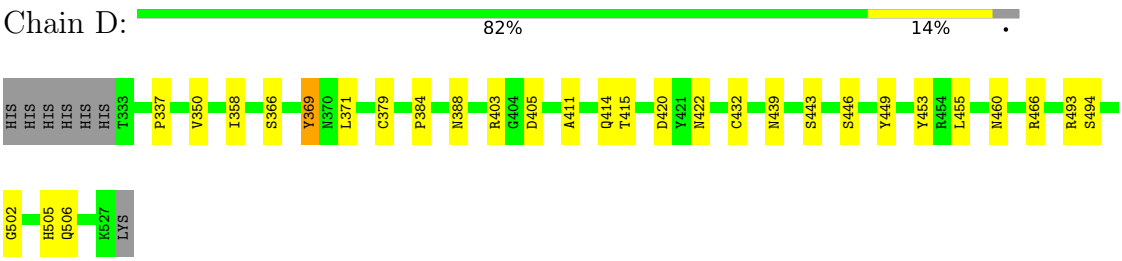
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Y	215	Total	C	N	O	S	0	1	0
			1646	1034	272	335	5			
5	T	215	Total	C	N	O	S	0	1	0
			1643	1033	272	333	5			
5	P	214	Total	C	N	O	S	0	1	0
			1635	1028	268	334	5			
5	R	215	Total	C	N	O	S	0	1	0
			1646	1034	272	335	5			

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

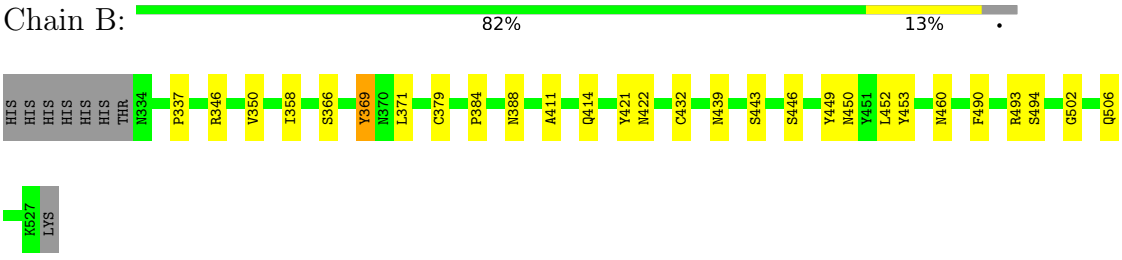
- Molecule 1: Spike protein S1

Chain D:



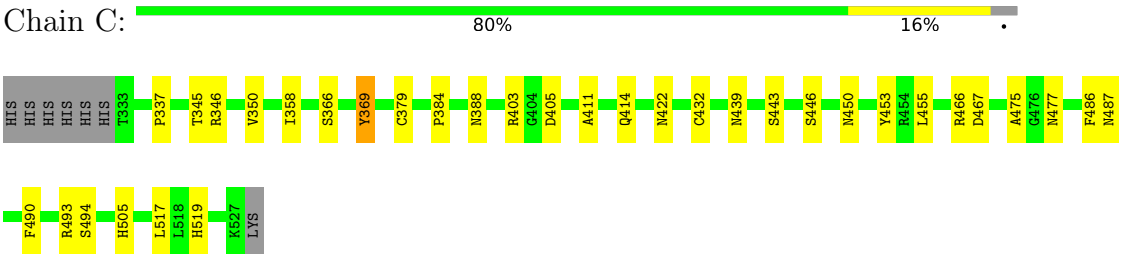
- Molecule 1: Spike protein S1

Chain B:



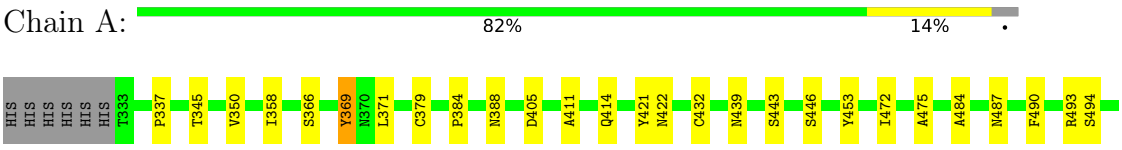
- Molecule 1: Spike protein S1

Chain C:



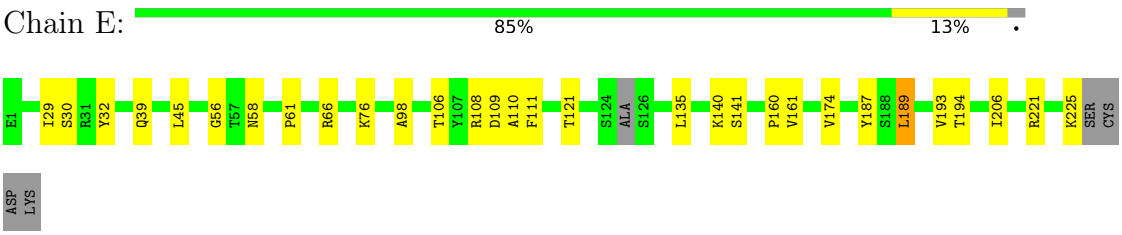
- Molecule 1: Spike protein S1

Chain A:



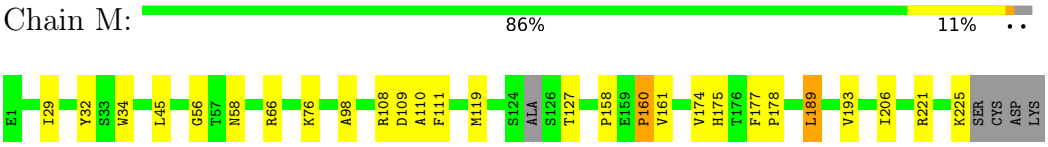
• Molecule 2: Omi-6 heavy chain

Chain E:



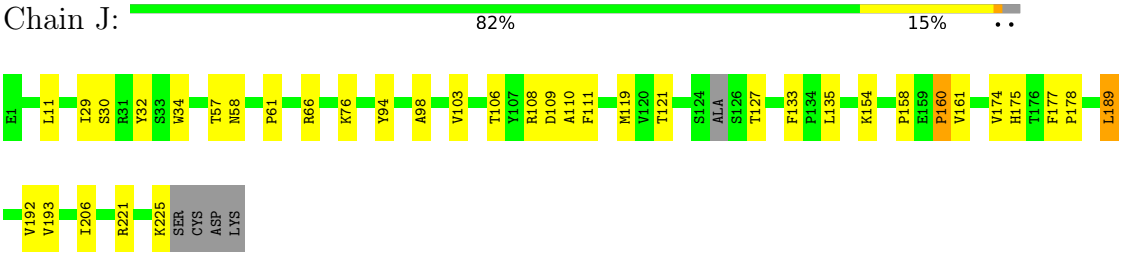
• Molecule 2: Omi-6 heavy chain

Chain M:



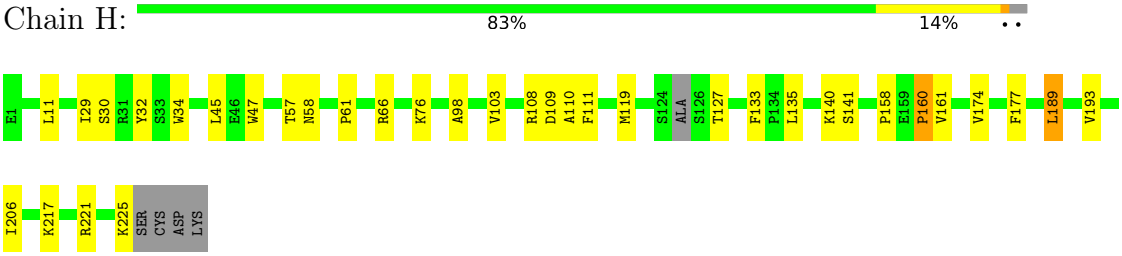
• Molecule 2: Omi-6 heavy chain

Chain J:



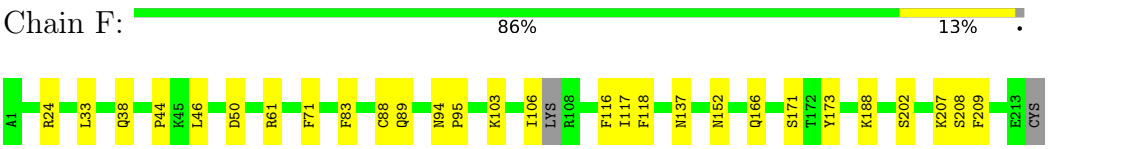
• Molecule 2: Omi-6 heavy chain

Chain H:



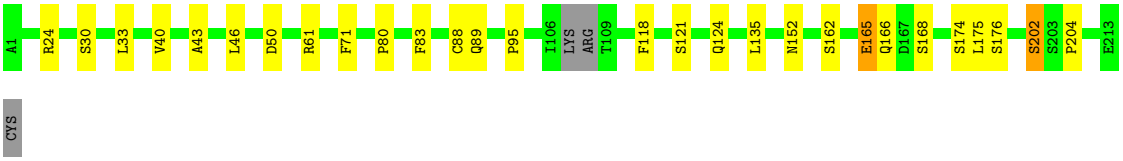
• Molecule 3: Omi-6 light chain

Chain F:



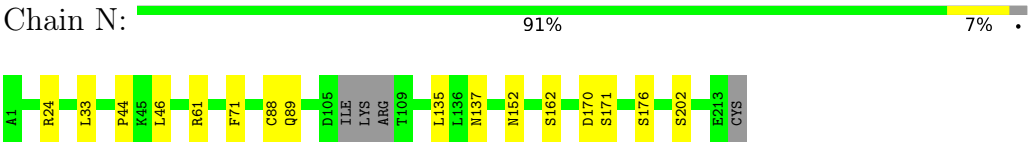
• Molecule 3: Omi-6 light chain

Chain K:



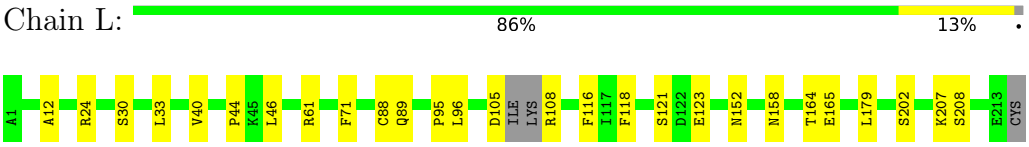
• Molecule 3: Omi-6 light chain

Chain N:



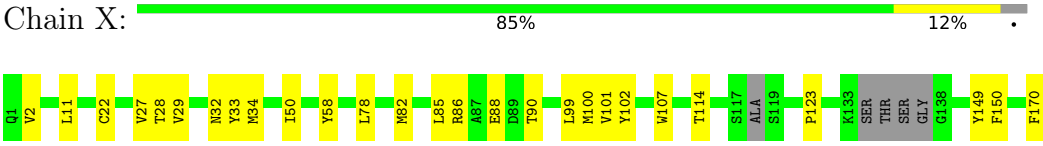
• Molecule 3: Omi-6 light chain

Chain L:



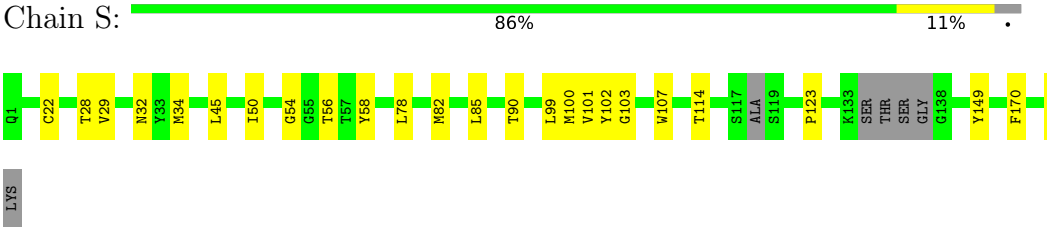
• Molecule 4: COVOX-150 heavy chain

Chain X:



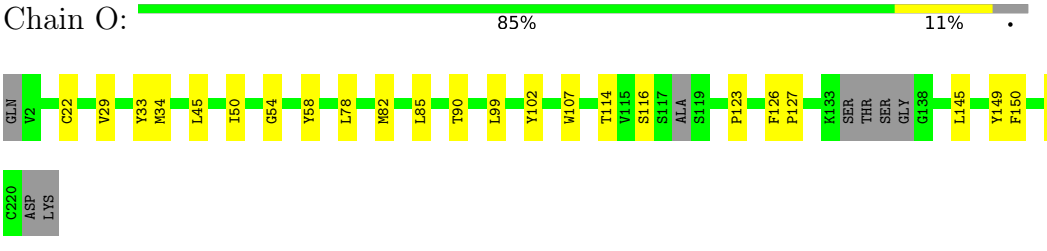
• Molecule 4: COVOX-150 heavy chain

Chain S:



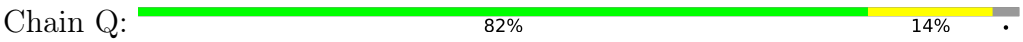
• Molecule 4: COVOX-150 heavy chain

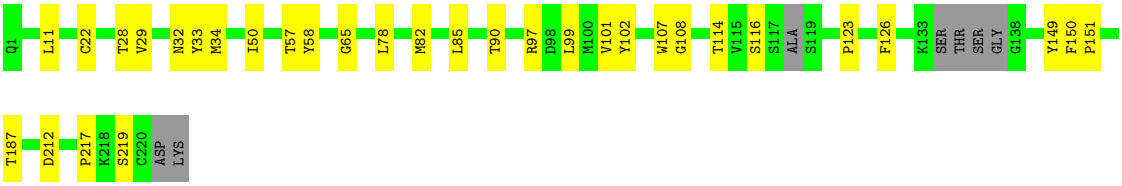
Chain O:



• Molecule 4: COVOX-150 heavy chain

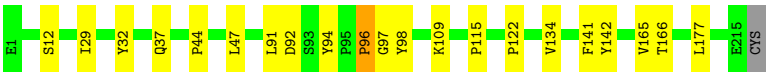
Chain Q:





• Molecule 5: COVOX-150 light chain

Chain Y:



• Molecule 5: COVOX-150 light chain

Chain T:

• Molecule 5: COVOX-150 light chain

Chain P:

• Molecule 5: COVOX-150 light chain

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.82Å 114.78Å 144.55Å 82.01° 80.62° 86.17°	Depositor
Resolution (Å)	113.55 – 4.24 113.55 – 4.24	Depositor EDS
% Data completeness (in resolution range)	34.0 (113.55-4.24) 34.0 (113.55-4.24)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 4.30Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.237 , 0.272 0.238 , 0.276	Depositor DCC
R_{free} test set	595 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.66	EDS
Total number of atoms	31966	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/1601	0.47	0/2179
1	B	0.26	0/1595	0.47	0/2171
1	C	0.26	0/1595	0.47	0/2171
1	D	0.26	0/1602	0.47	0/2181
2	E	0.56	0/1639	0.77	1/2238 (0.0%)
2	H	0.57	0/1650	0.77	1/2251 (0.0%)
2	J	0.57	0/1643	0.77	1/2242 (0.0%)
2	M	0.57	0/1650	0.77	1/2251 (0.0%)
3	F	0.58	0/1634	0.77	2/2215 (0.1%)
3	K	0.58	0/1624	0.76	2/2203 (0.1%)
3	L	0.57	0/1637	0.76	2/2219 (0.1%)
3	N	0.56	0/1613	0.78	3/2188 (0.1%)
4	O	0.25	0/1616	0.49	0/2201
4	Q	0.25	0/1625	0.49	0/2213
4	S	0.25	0/1625	0.49	0/2213
4	X	0.25	0/1625	0.49	0/2213
5	P	0.25	0/1673	0.49	0/2273
5	R	0.26	0/1685	0.60	3/2290 (0.1%)
5	T	0.28	0/1682	0.50	0/2286
5	Y	0.26	0/1685	0.65	3/2290 (0.1%)
All	All	0.41	0/32699	0.63	19/44488 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	109	LYS	O-C-N	14.73	146.26	122.70
5	R	109	LYS	O-C-N	-11.47	104.34	122.70
5	Y	109	LYS	CA-C-N	-11.41	92.09	117.20
5	R	109	LYS	C-N-CA	8.80	143.69	121.70
5	Y	109	LYS	C-N-CA	-8.52	100.41	121.70
5	R	109	LYS	CA-C-N	7.86	134.48	117.20
3	L	24	ARG	NE-CZ-NH2	-5.67	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	66	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	K	24	ARG	NE-CZ-NH2	-5.58	117.51	120.30
3	F	24	ARG	NE-CZ-NH2	-5.57	117.51	120.30
3	N	61	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	F	61	ARG	NE-CZ-NH1	5.55	123.07	120.30
3	N	24	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	M	66	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	H	66	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	J	66	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	K	61	ARG	NE-CZ-NH1	5.33	122.97	120.30
3	L	61	ARG	NE-CZ-NH1	5.29	122.95	120.30
3	N	24	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1556	0	1482	35	0
1	B	1550	0	1475	30	0
1	C	1551	0	1477	48	0
1	D	1557	0	1482	37	0
2	E	1605	0	1546	50	0
2	H	1615	0	1564	44	2
2	J	1608	0	1549	73	0
2	M	1615	0	1564	29	0
3	F	1603	0	1554	46	1
3	K	1592	0	1532	60	2
3	L	1604	0	1553	37	0
3	N	1581	0	1520	16	0
4	O	1583	0	1555	42	0
4	Q	1592	0	1567	28	2
4	S	1592	0	1567	33	0
4	X	1592	0	1567	23	0
5	P	1635	0	1593	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	1646	0	1607	25	0
5	T	1643	0	1605	35	1
5	Y	1646	0	1607	17	0
All	All	31966	0	30966	497	4

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 8.

All (497) 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:D:449:TYR:CE2	2:M:56:GLY:HA3	1.61	1.35
4:O:213:LYS:NZ	5:P:125:GLU:OE1	1.58	1.33
1:D:449:TYR:CZ	2:M:56:GLY:HA3	1.65	1.32
4:O:126:PHE:CZ	5:P:126:GLN:HG3	1.72	1.24
3:K:46:LEU:CD2	2:J:110:ALA:HB1	1.66	1.24
3:L:46:LEU:CD2	2:H:110:ALA:HB1	1.68	1.24
3:K:80:PRO:HB2	3:K:168:SER:O	1.38	1.23
4:O:126:PHE:CD1	5:P:126:GLN:HB2	1.76	1.19
2:E:45:LEU:HD11	3:F:44:PRO:CG	1.75	1.16
3:K:46:LEU:HD21	2:J:110:ALA:HB1	1.25	1.16
3:L:40:VAL:HG21	3:L:165:GLU:CB	1.79	1.12
1:B:449:TYR:CE2	2:E:56:GLY:HA3	1.84	1.12
3:K:135:LEU:CD1	2:J:177:PHE:HZ	1.64	1.10
3:L:12:ALA:HA	3:L:105:ASP:O	1.54	1.07
2:J:11:LEU:HD22	2:J:127:THR:HB	1.37	1.06
1:D:449:TYR:CZ	2:M:56:GLY:CA	2.38	1.05
5:T:109:LYS:HA	5:T:142:TYR:OH	1.54	1.05
3:K:135:LEU:HD22	2:J:192:VAL:HG21	1.37	1.05
3:L:46:LEU:HD21	2:H:110:ALA:HB1	1.32	1.04
4:O:126:PHE:CE2	5:P:126:GLN:HG3	1.95	1.02
1:B:449:TYR:CZ	2:E:56:GLY:HA3	1.94	1.01
3:K:80:PRO:CB	3:K:168:SER:O	2.09	1.00
3:L:46:LEU:HD22	2:H:110:ALA:HB1	1.42	0.97
3:K:46:LEU:HD22	2:J:110:ALA:HB1	1.49	0.95
4:O:213:LYS:CE	5:P:125:GLU:OE1	2.15	0.94
3:K:135:LEU:CD2	2:J:192:VAL:HG21	1.97	0.94
4:O:213:LYS:NZ	5:P:125:GLU:CD	2.20	0.94
2:E:45:LEU:CD1	3:F:44:PRO:HG2	1.98	0.93
3:K:135:LEU:CD1	2:J:177:PHE:CZ	2.50	0.93
3:K:162:SER:HB2	2:J:178:PRO:HB2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ASN:OD1	4:S:54:GLY:HA3	1.69	0.93
2:E:45:LEU:HD11	3:F:44:PRO:HG2	1.49	0.91
2:E:45:LEU:HD11	3:F:44:PRO:HG3	1.50	0.90
2:E:140:LYS:HD2	3:F:208:SER:O	1.70	0.90
3:K:40:VAL:HG21	3:K:165:GLU:HB2	1.53	0.90
4:O:126:PHE:CD1	5:P:126:GLN:CB	2.54	0.90
1:C:466:ARG:HH21	5:P:157:GLN:NE2	1.70	0.89
3:K:162:SER:CB	2:J:178:PRO:HB2	2.02	0.89
2:J:119:MET:HG2	2:J:160:PRO:HD3	1.54	0.89
3:L:207:LYS:HE2	2:H:140:LYS:O	1.75	0.87
3:K:135:LEU:HD13	2:J:177:PHE:CZ	2.09	0.87
1:B:346:ARG:NH1	3:F:50:ASP:OD1	2.08	0.86
5:R:109:LYS:HA	5:R:142:TYR:OH	1.75	0.86
2:H:206:ILE:HG12	2:H:221:ARG:HG2	1.58	0.85
1:D:449:TYR:CE2	2:M:56:GLY:CA	2.53	0.85
2:M:206:ILE:HG12	2:M:221:ARG:HG2	1.59	0.84
2:E:110:ALA:HB1	3:F:46:LEU:CD2	2.08	0.84
2:J:206:ILE:HG12	2:J:221:ARG:HG2	1.58	0.84
1:D:405:ASP:HB3	5:T:94:TYR:HB3	1.59	0.84
3:K:95:PRO:HB3	2:J:61:PRO:HD2	1.59	0.83
4:S:100:MET:O	5:T:91:LEU:HD22	1.79	0.83
2:E:206:ILE:HG12	2:E:221:ARG:HG2	1.58	0.83
2:M:127:THR:HG23	2:M:158:PRO:CD	2.08	0.83
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.61	0.83
1:D:449:TYR:OH	2:M:56:GLY:HA2	1.78	0.83
4:O:126:PHE:CE1	5:P:126:GLN:HG3	2.14	0.83
2:H:127:THR:HG23	2:H:158:PRO:CD	2.08	0.82
3:L:118:PHE:CD1	2:H:135:LEU:HB3	2.13	0.82
4:O:213:LYS:HZ2	5:P:125:GLU:CD	1.78	0.82
1:B:452:LEU:HG	2:E:106:THR:CB	2.09	0.82
3:F:33:LEU:HD11	3:F:88:CYS:HB2	1.61	0.82
1:C:446:SER:HB2	2:J:58:ASN:HA	1.59	0.82
4:O:116:SER:HB3	4:O:150:PHE:CZ	2.15	0.81
1:D:460:ASN:ND2	4:S:54:GLY:O	2.12	0.81
3:N:33:LEU:HD11	3:N:88:CYS:HB2	1.61	0.81
1:C:345:THR:HG21	3:K:30:SER:OG	1.80	0.81
2:E:110:ALA:HB1	3:F:46:LEU:HD22	1.62	0.81
3:K:33:LEU:HD11	3:K:88:CYS:HB2	1.61	0.80
4:Q:116:SER:HB3	4:Q:150:PHE:CZ	2.17	0.80
4:O:126:PHE:CE1	5:P:126:GLN:HA	2.15	0.80
3:L:158:ASN:ND2	3:L:179:LEU:HD11	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:175:LEU:C	2:J:177:PHE:CE1	2.56	0.79
1:A:345:THR:HG21	3:L:30:SER:OG	1.83	0.79
3:L:158:ASN:HD22	3:L:179:LEU:HD11	1.47	0.79
1:A:490:PHE:CG	2:H:30:SER:HB2	2.17	0.79
1:D:449:TYR:OH	2:M:56:GLY:CA	2.31	0.78
4:S:101:VAL:O	5:T:49:TYR:HB2	1.82	0.78
1:D:403:ARG:NH2	5:T:92:ASP:OD1	2.15	0.78
1:B:449:TYR:OH	2:E:56:GLY:CA	2.31	0.78
1:A:405:ASP:CG	5:R:94:TYR:CD2	2.58	0.77
2:E:140:LYS:CD	3:F:208:SER:O	2.32	0.77
3:K:162:SER:HB2	2:J:178:PRO:CB	2.14	0.77
1:C:453:TYR:OH	1:C:493:ARG:HD3	1.85	0.77
1:A:453:TYR:OH	1:A:493:ARG:HD3	1.85	0.77
4:S:102:TYR:O	5:T:46:LEU:HD21	1.85	0.76
1:D:453:TYR:OH	1:D:493:ARG:HD3	1.85	0.76
3:N:33:LEU:HD22	3:N:71:PHE:CG	2.21	0.76
4:O:126:PHE:CE1	5:P:126:GLN:CB	2.69	0.76
3:L:95:PRO:HB3	2:H:61:PRO:HD2	1.67	0.76
1:D:505:HIS:NE2	5:T:29:ILE:HA	2.01	0.75
3:K:162:SER:OG	2:J:178:PRO:HD2	1.86	0.75
3:L:46:LEU:CD2	2:H:110:ALA:CB	2.58	0.75
3:F:33:LEU:HD22	3:F:71:PHE:CG	2.21	0.75
1:C:466:ARG:NH2	5:P:157:GLN:NE2	2.34	0.75
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.21	0.75
3:L:46:LEU:HD21	2:H:110:ALA:CB	2.16	0.75
1:B:453:TYR:OH	1:B:493:ARG:HD3	1.85	0.74
3:K:33:LEU:HD22	3:K:71:PHE:CG	2.22	0.74
2:H:127:THR:HG23	2:H:158:PRO:HD2	1.70	0.74
1:C:519:HIS:CB	4:Q:217:PRO:HG2	2.17	0.74
1:D:405:ASP:HB3	5:T:94:TYR:CB	2.17	0.74
1:C:466:ARG:HH21	5:P:157:GLN:HE22	1.31	0.74
4:S:103:GLY:HA3	5:T:46:LEU:CD2	2.18	0.74
4:S:103:GLY:HA3	5:T:46:LEU:HD22	1.69	0.74
2:E:140:LYS:O	3:F:207:LYS:HE2	1.87	0.74
1:B:490:PHE:CB	2:E:30:SER:CB	2.66	0.74
2:M:127:THR:HG23	2:M:158:PRO:HD2	1.70	0.74
3:L:40:VAL:HG11	3:L:165:GLU:CB	2.18	0.73
4:S:107:TRP:CE3	5:T:44:PRO:HD2	2.22	0.73
1:C:475:ALA:HB1	4:X:32:ASN:OD1	1.88	0.73
3:K:135:LEU:HD12	2:J:177:PHE:HZ	1.51	0.73
4:Q:107:TRP:CE3	5:R:44:PRO:HD2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ALA:HB2	1:A:490:PHE:CE2	2.24	0.73
3:K:95:PRO:HB3	2:J:61:PRO:CD	2.18	0.73
4:O:126:PHE:CG	5:P:126:GLN:HB2	2.23	0.73
1:A:490:PHE:CD1	2:H:30:SER:HB3	2.24	0.72
3:K:176:SER:HB3	2:J:177:PHE:CE2	2.24	0.72
1:C:493:ARG:HD2	4:X:101:VAL:HG21	1.70	0.72
1:B:449:TYR:CZ	2:E:56:GLY:CA	2.73	0.71
1:B:449:TYR:OH	2:E:56:GLY:HA3	1.90	0.71
2:E:140:LYS:CE	3:F:208:SER:O	2.38	0.71
3:K:176:SER:N	2:J:177:PHE:CE1	2.58	0.71
1:B:446:SER:HB3	2:E:58:ASN:CB	2.22	0.70
1:B:450:ASN:O	2:E:106:THR:CB	2.39	0.70
4:X:29:VAL:HG13	4:X:34:MET:HG3	1.74	0.70
3:K:124:GLN:NE2	2:J:154:LYS:HE3	2.05	0.70
2:M:127:THR:HG23	2:M:158:PRO:HD3	1.74	0.70
4:O:29:VAL:HG13	4:O:34:MET:HG3	1.74	0.70
1:A:405:ASP:HB3	5:R:94:TYR:CB	2.22	0.69
4:S:29:VAL:HG13	4:S:34:MET:HG3	1.74	0.69
1:C:490:PHE:CD2	2:J:30:SER:OG	2.45	0.69
2:H:127:THR:HG23	2:H:158:PRO:HD3	1.74	0.69
4:O:213:LYS:HE2	5:P:125:GLU:OE1	1.91	0.69
4:Q:29:VAL:HG13	4:Q:34:MET:HG3	1.74	0.68
1:C:405:ASP:HB3	5:Y:94:TYR:HB3	1.75	0.68
1:A:490:PHE:CD1	2:H:30:SER:CB	2.76	0.68
2:E:45:LEU:CD1	3:F:44:PRO:CG	2.56	0.68
3:K:118:PHE:CD1	2:J:135:LEU:HB3	2.29	0.68
3:L:46:LEU:HD22	2:H:110:ALA:CB	2.19	0.67
3:K:176:SER:HB3	2:J:177:PHE:CD2	2.30	0.67
1:C:490:PHE:CD2	2:J:30:SER:HB3	2.29	0.67
1:C:405:ASP:HB3	5:Y:94:TYR:CB	2.23	0.67
4:O:126:PHE:CE1	5:P:126:GLN:CA	2.77	0.67
3:N:33:LEU:CD2	3:N:71:PHE:CG	2.79	0.66
3:K:162:SER:HB2	2:J:178:PRO:CG	2.25	0.66
2:M:45:LEU:HD11	3:N:44:PRO:HG2	1.77	0.66
3:L:33:LEU:CD2	3:L:71:PHE:CG	2.78	0.66
4:S:107:TRP:CH2	5:T:44:PRO:HG2	2.29	0.66
3:K:33:LEU:CD2	3:K:71:PHE:CG	2.79	0.66
3:F:33:LEU:CD2	3:F:71:PHE:CG	2.79	0.66
1:C:446:SER:CB	2:J:58:ASN:HA	2.25	0.66
1:C:490:PHE:CG	2:J:30:SER:HB3	2.30	0.66
1:D:366:SER:HA	1:D:369:TYR:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ALA:HB1	4:Q:32:ASN:OD1	1.96	0.65
3:K:162:SER:OG	2:J:178:PRO:CD	2.44	0.65
1:C:366:SER:HA	1:C:369:TYR:HB2	1.78	0.65
1:A:366:SER:HA	1:A:369:TYR:HB2	1.78	0.65
4:O:126:PHE:CE1	5:P:126:GLN:CG	2.80	0.65
1:A:472:ILE:HD11	1:A:490:PHE:CE1	2.31	0.64
3:L:40:VAL:CG2	3:L:165:GLU:CB	2.68	0.64
3:K:83:PHE:CB	3:K:166:GLN:HE21	2.11	0.64
1:C:490:PHE:CD2	2:J:30:SER:CB	2.80	0.64
5:T:109:LYS:HA	5:T:142:TYR:HH	1.63	0.64
5:P:109:LYS:HA	5:P:142:TYR:OH	1.98	0.64
1:B:366:SER:HA	1:B:369:TYR:HB2	1.78	0.63
4:S:102:TYR:O	5:T:46:LEU:CD2	2.46	0.63
1:A:490:PHE:CG	2:H:30:SER:CB	2.81	0.63
3:L:95:PRO:HB3	2:H:61:PRO:CD	2.29	0.63
3:L:158:ASN:ND2	3:L:179:LEU:CD1	2.61	0.63
2:H:108:ARG:O	2:H:110:ALA:N	2.33	0.62
1:C:517:LEU:O	4:Q:219:SER:OG	2.17	0.62
3:K:83:PHE:HB3	3:K:166:GLN:NE2	2.14	0.62
2:M:108:ARG:O	2:M:110:ALA:N	2.33	0.62
4:O:127:PRO:HD2	5:P:123:SER:CB	2.30	0.62
3:F:106:ILE:HG22	3:F:166:GLN:NE2	2.15	0.62
5:P:122:PRO:HD3	5:P:134:VAL:HG22	1.81	0.62
2:E:108:ARG:O	2:E:110:ALA:N	2.33	0.62
2:J:108:ARG:O	2:J:110:ALA:N	2.33	0.61
1:C:477:ASN:HD21	5:P:3:VAL:HG22	1.65	0.61
3:K:135:LEU:HD13	2:J:177:PHE:CE2	2.34	0.61
1:D:439:ASN:O	1:D:443:SER:OG	2.18	0.61
3:K:33:LEU:HD12	3:K:89:GLN:O	2.01	0.61
3:F:33:LEU:HD12	3:F:89:GLN:O	2.01	0.61
4:Q:116:SER:HB3	4:Q:150:PHE:HZ	1.66	0.61
1:C:439:ASN:O	1:C:443:SER:OG	2.18	0.61
5:T:122:PRO:HD3	5:T:134:VAL:HG22	1.81	0.61
1:B:446:SER:HB2	3:F:94:ASN:ND2	2.16	0.61
2:E:140:LYS:HG3	3:F:209:PHE:HB3	1.81	0.61
3:N:33:LEU:HD12	3:N:89:GLN:O	2.01	0.61
5:Y:122:PRO:HD3	5:Y:134:VAL:HG22	1.81	0.61
3:F:106:ILE:HD13	3:F:171:SER:OG	1.99	0.61
3:L:33:LEU:HD12	3:L:89:GLN:O	2.01	0.60
1:A:439:ASN:O	1:A:443:SER:OG	2.18	0.60
4:O:126:PHE:CE2	5:P:126:GLN:CG	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:122:PRO:HD3	5:R:134:VAL:HG22	1.81	0.60
2:M:45:LEU:HD11	3:N:44:PRO:CG	2.31	0.60
3:K:46:LEU:HD22	2:J:110:ALA:CB	2.29	0.60
3:K:175:LEU:C	2:J:177:PHE:HE1	2.04	0.60
2:E:110:ALA:HB1	3:F:46:LEU:HD21	1.82	0.60
2:E:140:LYS:HB3	3:F:117:ILE:CG2	2.32	0.60
2:E:39:GLN:CD	3:F:38:GLN:HE22	2.05	0.60
3:K:135:LEU:HD22	2:J:192:VAL:CG2	2.24	0.60
3:K:176:SER:HB3	2:J:177:PHE:CZ	2.37	0.59
1:C:446:SER:O	2:J:57:THR:O	2.19	0.59
3:L:12:ALA:CA	3:L:105:ASP:O	2.41	0.59
4:Q:22:CYS:HB3	4:Q:78:LEU:HB3	1.85	0.59
2:J:119:MET:HG2	2:J:160:PRO:CD	2.30	0.59
3:F:103:LYS:NZ	3:F:173:TYR:OH	2.36	0.59
5:P:187:ASP:OD1	2:J:103:VAL:CB	2.51	0.59
2:J:32:TYR:HD2	2:J:98:ALA:O	1.86	0.59
1:C:455:LEU:HD11	4:X:100:MET:HG3	1.85	0.59
3:K:46:LEU:HD21	2:J:110:ALA:CB	2.16	0.59
4:X:22:CYS:HB3	4:X:78:LEU:HB3	1.85	0.59
4:X:11:LEU:HD21	4:X:150:PHE:CE2	2.38	0.58
2:M:32:TYR:HD2	2:M:98:ALA:O	1.86	0.58
1:B:439:ASN:O	1:B:443:SER:OG	2.18	0.58
2:E:121:THR:HG21	2:E:187:TYR:OH	2.04	0.58
3:K:162:SER:HB2	2:J:178:PRO:HG2	1.85	0.58
3:L:33:LEU:CD2	3:L:71:PHE:CB	2.82	0.58
4:O:116:SER:HB3	4:O:150:PHE:HZ	1.69	0.58
2:H:32:TYR:HD2	2:H:98:ALA:O	1.86	0.58
4:O:22:CYS:HB3	4:O:78:LEU:HB3	1.85	0.58
2:H:119:MET:HB3	2:H:160:PRO:HD3	1.86	0.57
1:C:405:ASP:CG	5:Y:94:TYR:CD2	2.78	0.57
1:A:405:ASP:HB3	5:R:94:TYR:HB3	1.85	0.57
1:C:519:HIS:CB	4:Q:217:PRO:CG	2.82	0.57
4:S:22:CYS:HB3	4:S:78:LEU:HB3	1.85	0.57
4:O:175:GLN:HG2	5:P:162:GLN:OE1	2.04	0.57
3:F:33:LEU:CD2	3:F:71:PHE:CB	2.82	0.57
4:X:107:TRP:CE3	5:Y:44:PRO:HD2	2.38	0.57
3:K:83:PHE:HB3	3:K:166:GLN:HE21	1.68	0.57
2:J:121:THR:HG21	2:J:158:PRO:HG3	1.87	0.57
1:A:446:SER:HB2	2:H:58:ASN:HA	1.85	0.57
3:K:33:LEU:CD2	3:K:71:PHE:CB	2.82	0.57
1:D:466:ARG:NH2	5:R:157:GLN:NE2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ARG:NH2	5:P:157:GLN:HE22	1.98	0.56
4:S:170:PHE:HB3	5:T:164:SER:OG	2.05	0.56
1:D:405:ASP:CB	5:T:94:TYR:HB3	2.34	0.56
2:E:32:TYR:HD2	2:E:98:ALA:O	1.86	0.56
3:N:33:LEU:CD2	3:N:71:PHE:CB	2.82	0.56
4:X:86:ARG:HD2	4:X:88:GLU:OE2	2.04	0.56
1:C:446:SER:OG	2:J:58:ASN:CB	2.53	0.56
3:K:162:SER:CB	2:J:178:PRO:CB	2.77	0.56
1:B:490:PHE:CB	2:E:30:SER:HB2	2.34	0.56
3:K:43:ALA:HB2	2:J:94:TYR:CE1	2.41	0.55
3:K:174:SER:OG	2:J:175:HIS:CE1	2.59	0.55
3:L:44:PRO:CG	2:H:45:LEU:HD11	2.36	0.55
3:L:208:SER:O	2:H:140:LYS:HD2	2.06	0.55
2:E:39:GLN:HE22	3:F:38:GLN:CD	2.10	0.55
2:M:174:VAL:HG22	2:M:193:VAL:HG22	1.89	0.55
2:E:174:VAL:HG22	2:E:193:VAL:HG22	1.89	0.55
2:J:174:VAL:HG22	2:J:193:VAL:HG22	1.89	0.55
2:E:39:GLN:OE1	3:F:38:GLN:NE2	2.32	0.55
2:M:175:HIS:CD2	3:N:137:ASN:OD1	2.60	0.55
4:Q:90:THR:HG23	4:Q:114:THR:HA	1.89	0.55
2:E:135:LEU:HB3	3:F:118:PHE:CD1	2.42	0.55
2:H:174:VAL:HG22	2:H:193:VAL:HG22	1.88	0.55
1:D:405:ASP:CG	5:T:94:TYR:CD2	2.80	0.54
1:C:446:SER:HB2	2:J:57:THR:O	2.08	0.54
3:L:118:PHE:CE1	2:H:135:LEU:HB3	2.42	0.54
5:P:37:GLN:HB2	5:P:47:LEU:HD11	1.90	0.54
1:A:405:ASP:OD1	5:R:94:TYR:CD2	2.61	0.54
3:K:175:LEU:CA	2:J:177:PHE:HE1	2.21	0.54
4:O:145:LEU:CD2	5:P:133:SER:CB	2.85	0.54
1:D:466:ARG:NH2	5:R:157:GLN:HE22	2.05	0.54
4:X:90:THR:HG23	4:X:114:THR:HA	1.89	0.54
1:B:449:TYR:HE2	2:E:56:GLY:HA3	1.61	0.54
4:S:90:THR:HG23	4:S:114:THR:HA	1.89	0.53
5:T:37:GLN:HB2	5:T:47:LEU:HD11	1.89	0.53
1:A:484:ALA:HB2	1:A:490:PHE:CZ	2.43	0.53
3:F:106:ILE:HG22	3:F:166:GLN:CD	2.28	0.53
4:O:90:THR:HG23	4:O:114:THR:HA	1.89	0.53
3:K:166:GLN:OE1	3:K:166:GLN:N	2.36	0.53
4:O:127:PRO:HD2	5:P:123:SER:OG	2.09	0.53
5:R:37:GLN:HB2	5:R:47:LEU:HD11	1.90	0.53
2:M:110:ALA:HB1	3:N:46:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:MET:HB3	2:M:160:PRO:HD3	1.90	0.52
1:A:484:ALA:CB	1:A:490:PHE:CE2	2.91	0.52
2:E:45:LEU:HD13	3:F:44:PRO:HG2	1.85	0.52
5:Y:37:GLN:HB2	5:Y:47:LEU:HD11	1.90	0.52
4:S:107:TRP:CD2	5:T:44:PRO:HD2	2.44	0.52
3:K:80:PRO:HB3	3:K:168:SER:O	2.05	0.52
1:D:466:ARG:HH21	5:R:157:GLN:NE2	2.08	0.52
3:F:106:ILE:HG23	3:F:106:ILE:O	2.10	0.52
1:D:466:ARG:HH21	5:R:157:GLN:HE22	1.59	0.51
4:S:45:LEU:HD11	5:T:44:PRO:HG3	1.92	0.51
2:E:39:GLN:NE2	3:F:38:GLN:HE22	2.08	0.51
1:A:490:PHE:CD1	2:H:30:SER:HB2	2.42	0.51
1:D:455:LEU:HD11	4:S:100:MET:HG3	1.93	0.51
4:X:82:MET:HB3	4:X:85:LEU:HD21	1.93	0.51
4:O:123:PRO:HB3	4:O:149:TYR:HB3	1.93	0.51
4:X:123:PRO:HB3	4:X:149:TYR:HB3	1.93	0.51
1:D:415:THR:HB	4:S:56:THR:OG1	2.10	0.51
3:F:106:ILE:CG2	3:F:166:GLN:NE2	2.73	0.51
3:K:118:PHE:HB3	2:J:135:LEU:HD22	1.93	0.51
3:K:124:GLN:HE21	2:J:154:LYS:HE3	1.75	0.51
4:O:82:MET:HB3	4:O:85:LEU:HD21	1.93	0.51
2:E:39:GLN:HE22	3:F:38:GLN:NE2	2.09	0.50
4:S:82:MET:HB3	4:S:85:LEU:HD21	1.93	0.50
2:E:61:PRO:HD2	3:F:95:PRO:HB3	1.93	0.50
3:L:96:LEU:HD12	2:H:47:TRP:CE2	2.46	0.50
2:J:119:MET:CG	2:J:160:PRO:HD3	2.37	0.50
4:Q:123:PRO:HB3	4:Q:149:TYR:HB3	1.93	0.50
1:B:490:PHE:CB	2:E:30:SER:OG	2.59	0.50
3:L:123:GLU:HB2	2:H:133:PHE:HD1	1.75	0.50
4:X:99:LEU:HB3	4:X:102:TYR:HB2	1.94	0.50
4:S:123:PRO:HB3	4:S:149:TYR:HB3	1.93	0.49
4:Q:82:MET:HB3	4:Q:85:LEU:HD21	1.93	0.49
1:C:493:ARG:CD	4:X:101:VAL:HG21	2.40	0.49
3:K:176:SER:HB3	2:J:177:PHE:CG	2.47	0.49
4:Q:99:LEU:HB3	4:Q:102:TYR:HB2	1.94	0.49
4:S:99:LEU:HB3	4:S:102:TYR:HB2	1.94	0.49
5:T:165[A]:VAL:HG22	5:T:177:LEU:HD12	1.94	0.49
4:Q:11:LEU:HD22	4:Q:151:PRO:HG3	1.94	0.49
5:R:165[A]:VAL:HG22	5:R:177:LEU:HD12	1.95	0.49
1:B:460:ASN:OD1	4:O:54:GLY:HA3	2.12	0.49
5:P:115:PRO:HB3	5:P:141:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:165[A]:VAL:HG22	5:P:177:LEU:HD12	1.94	0.48
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.53	0.48
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.53	0.48
4:O:145:LEU:CD2	5:P:133:SER:HB2	2.42	0.48
4:Q:187:THR:HG21	5:R:139:ASN:ND2	2.28	0.48
2:E:39:GLN:NE2	3:F:38:GLN:OE1	2.38	0.48
4:O:99:LEU:HB3	4:O:102:TYR:HB2	1.94	0.48
1:D:350:VAL:HG22	1:D:422:ASN:HB3	1.96	0.48
1:C:403:ARG:NH2	5:Y:92:ASP:OD1	2.47	0.48
1:A:405:ASP:HB3	5:R:94:TYR:CG	2.48	0.48
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.96	0.48
2:M:178:PRO:HB2	3:N:162:SER:HB2	1.94	0.48
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.48
3:K:135:LEU:HD12	2:J:177:PHE:CZ	2.34	0.48
5:Y:165[A]:VAL:HG22	5:Y:177:LEU:HD12	1.94	0.48
5:T:165[B]:VAL:HG22	5:T:177:LEU:HD12	1.96	0.48
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.96	0.48
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.53	0.48
3:L:121:SER:OG	2:H:133:PHE:HB3	2.14	0.48
4:O:126:PHE:CZ	5:P:126:GLN:CG	2.66	0.48
5:R:165[B]:VAL:HG22	5:R:177:LEU:HD12	1.96	0.48
2:M:110:ALA:HB1	3:N:46:LEU:CD2	2.44	0.47
4:Q:108:GLY:O	5:R:43:ALA:HB2	2.14	0.47
1:C:450:ASN:O	2:J:106:THR:CB	2.62	0.47
1:A:493:ARG:HD2	4:Q:101:VAL:HG21	1.96	0.47
2:J:121:THR:CB	2:J:158:PRO:HG3	2.44	0.47
5:T:115:PRO:HB3	5:T:141:PHE:HB3	1.96	0.47
4:O:213:LYS:NZ	5:P:125:GLU:OE2	2.47	0.47
1:D:379:CYS:SG	1:D:384:PRO:HG3	2.53	0.47
4:S:187:THR:HG21	5:T:139:ASN:ND2	2.29	0.47
5:Y:115:PRO:HB3	5:Y:141:PHE:HB3	1.96	0.47
1:C:466:ARG:NH2	5:P:157:GLN:HE21	2.13	0.47
4:O:126:PHE:HE1	5:P:126:GLN:HA	1.73	0.47
5:R:115:PRO:HB3	5:R:141:PHE:HB3	1.96	0.47
4:S:107:TRP:CB	5:T:43:ALA:HB1	2.45	0.46
3:K:176:SER:N	2:J:177:PHE:CD1	2.83	0.46
5:P:165[B]:VAL:HG22	5:P:177:LEU:HD12	1.96	0.46
5:Y:165[B]:VAL:HG22	5:Y:177:LEU:HD12	1.96	0.46
2:H:32:TYR:CD2	2:H:98:ALA:O	2.68	0.46
2:E:32:TYR:CD2	2:E:98:ALA:O	2.68	0.46
4:X:50:ILE:HG22	4:X:58:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:95:PRO:CB	2:H:61:PRO:HD2	2.43	0.46
4:X:11:LEU:HD11	4:X:150:PHE:HZ	1.80	0.46
1:B:449:TYR:OH	2:E:56:GLY:HA2	2.12	0.46
4:O:127:PRO:HG2	5:P:123:SER:HB3	1.98	0.45
2:E:29:ILE:CD1	2:E:76:LYS:HA	2.47	0.45
4:O:107:TRP:CE3	5:P:44:PRO:HD2	2.51	0.45
1:C:455:LEU:HD21	4:X:100:MET:HB2	1.97	0.45
3:F:33:LEU:HD22	3:F:71:PHE:CD1	2.52	0.45
2:M:29:ILE:CD1	2:M:76:LYS:HA	2.47	0.45
2:M:127:THR:CG2	2:M:158:PRO:HD2	2.44	0.45
2:E:141:SER:C	3:F:116:PHE:HD2	2.19	0.45
4:O:50:ILE:HG22	4:O:58:TYR:HB2	1.98	0.45
5:P:204:SER:HB2	4:Q:212:ASP:HB2	1.98	0.45
4:Q:50:ILE:HG22	4:Q:58:TYR:HB2	1.98	0.45
2:J:29:ILE:CD1	2:J:76:LYS:HA	2.47	0.45
2:H:127:THR:CG2	2:H:158:PRO:HD2	2.44	0.45
3:K:118:PHE:CB	2:J:135:LEU:HD22	2.46	0.45
1:B:421:TYR:HE2	4:O:33:TYR:OH	2.00	0.45
1:C:346:ARG:NH1	3:K:50:ASP:OD1	2.50	0.45
2:M:177:PHE:CE2	3:N:176:SER:HB3	2.51	0.45
2:H:29:ILE:CD1	2:H:76:LYS:HA	2.47	0.45
2:M:177:PHE:HZ	3:N:135:LEU:CD1	2.29	0.45
3:L:33:LEU:HD22	3:L:71:PHE:CD1	2.52	0.45
3:L:123:GLU:HB2	2:H:133:PHE:CD1	2.52	0.45
5:T:108:ILE:O	5:T:168:GLN:NE2	2.43	0.45
2:J:32:TYR:CD2	2:J:98:ALA:O	2.68	0.44
3:L:44:PRO:HG3	2:H:45:LEU:HD11	1.98	0.44
1:C:446:SER:HB2	2:J:58:ASN:CA	2.39	0.44
3:K:121:SER:OG	2:J:133:PHE:HB3	2.17	0.44
3:L:118:PHE:CB	2:H:135:LEU:HD22	2.47	0.44
4:O:34:MET:HB3	4:O:78:LEU:HD22	2.00	0.44
3:K:33:LEU:HD22	3:K:71:PHE:CD1	2.52	0.44
3:K:40:VAL:HG21	3:K:165:GLU:CB	2.38	0.44
1:B:493:ARG:HG2	1:B:494:SER:N	2.33	0.44
4:S:34:MET:HB3	4:S:78:LEU:HD22	2.00	0.44
4:S:50:ILE:HG22	4:S:58:TYR:HB2	1.98	0.44
1:C:405:ASP:CB	5:Y:94:TYR:HB3	2.44	0.44
1:A:472:ILE:CD1	1:A:490:PHE:CD1	3.00	0.44
2:E:140:LYS:HB3	3:F:117:ILE:HG22	2.00	0.44
4:X:34:MET:HB3	4:X:78:LEU:HD22	2.00	0.44
4:O:45:LEU:HD11	5:P:44:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:LEU:HD23	1:D:371:LEU:HA	1.88	0.44
2:E:140:LYS:HE3	3:F:208:SER:O	2.16	0.44
3:K:176:SER:HB3	2:J:177:PHE:CE1	2.53	0.44
2:M:161:VAL:CG2	2:M:189:LEU:HD13	2.48	0.44
4:X:28:THR:O	4:X:32:ASN:ND2	2.49	0.44
1:D:493:ARG:HG2	1:D:494:SER:N	2.33	0.43
1:A:405:ASP:CB	5:R:94:TYR:HB3	2.47	0.43
3:N:33:LEU:HD22	3:N:71:PHE:CD1	2.52	0.43
5:T:96:PRO:O	5:T:98:TYR:N	2.51	0.43
1:D:446:SER:HB2	2:M:58:ASN:HA	2.00	0.43
1:A:446:SER:O	2:H:57:THR:O	2.37	0.43
1:A:493:ARG:HG2	1:A:494:SER:N	2.33	0.43
2:H:161:VAL:CG2	2:H:189:LEU:HD13	2.48	0.43
1:C:493:ARG:HG2	1:C:494:SER:N	2.33	0.43
5:R:96:PRO:O	5:R:98:TYR:N	2.51	0.43
2:J:121:THR:HG21	2:J:158:PRO:CB	2.47	0.43
5:Y:96:PRO:O	5:Y:98:TYR:N	2.51	0.43
2:M:32:TYR:CD2	2:M:98:ALA:O	2.68	0.43
4:S:102:TYR:HA	5:T:49:TYR:CG	2.53	0.43
4:Q:28:THR:O	4:Q:32:ASN:ND2	2.49	0.43
4:Q:34:MET:HB3	4:Q:78:LEU:HD22	2.00	0.43
2:M:206:ILE:CG1	2:M:221:ARG:HG2	2.41	0.43
1:D:420:ASP:OD2	4:S:56:THR:OG1	2.24	0.43
2:J:206:ILE:CG1	2:J:221:ARG:HG2	2.40	0.43
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.88	0.43
2:E:161:VAL:CG2	2:E:189:LEU:HD13	2.48	0.43
4:Q:107:TRP:HB3	5:R:43:ALA:HB1	2.00	0.43
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.01	0.42
5:Y:12:SER:OG	5:Y:142:TYR:OH	2.30	0.42
3:F:106:ILE:CG2	3:F:171:SER:HB3	2.49	0.42
1:D:411:ALA:HB3	1:D:414:GLN:HG3	2.01	0.42
1:A:487:ASN:OD1	4:Q:97:ARG:NH2	2.30	0.42
2:J:161:VAL:CG2	2:J:189:LEU:HD13	2.48	0.42
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.02	0.42
3:L:116:PHE:HD2	2:H:141:SER:HA	1.84	0.42
1:D:379:CYS:HA	1:D:432:CYS:HA	2.02	0.42
1:A:379:CYS:HA	1:A:432:CYS:HA	2.02	0.42
4:S:103:GLY:HA3	5:T:46:LEU:HD21	1.99	0.42
4:O:116:SER:CB	4:O:150:PHE:CZ	2.95	0.42
1:B:369:TYR:OH	1:B:388:ASN:ND2	2.52	0.42
1:A:421:TYR:HE2	4:Q:33:TYR:OH	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:107:TRP:CZ2	5:T:44:PRO:HB2	2.54	0.42
1:C:369:TYR:OH	1:C:388:ASN:ND2	2.53	0.42
3:N:170:ASP:O	3:N:171:SER:OG	2.34	0.42
4:S:28:THR:O	4:S:32:ASN:ND2	2.49	0.42
4:S:107:TRP:CZ3	5:T:44:PRO:HG2	2.55	0.42
2:E:61:PRO:CD	3:F:95:PRO:HB3	2.49	0.42
3:F:83:PHE:CE1	3:F:106:ILE:HA	2.55	0.42
4:O:145:LEU:HD21	5:P:133:SER:CB	2.49	0.42
4:Q:126:PHE:CD1	5:R:126:GLN:HB2	2.55	0.42
1:C:467:ASP:HA	5:P:158:SER:OG	2.20	0.42
3:K:135:LEU:HD21	2:J:192:VAL:HG21	1.94	0.42
1:C:379:CYS:HA	1:C:432:CYS:HA	2.02	0.41
4:Q:126:PHE:CE2	5:R:126:GLN:HG3	2.55	0.41
1:B:446:SER:HB2	3:F:94:ASN:HD22	1.82	0.41
5:T:109:LYS:HA	5:T:142:TYR:CZ	2.50	0.41
1:C:411:ALA:HB3	1:C:414:GLN:HG3	2.02	0.41
3:L:164:THR:HG23	2:H:177:PHE:CD1	2.56	0.41
2:H:206:ILE:CG1	2:H:221:ARG:HG2	2.40	0.41
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.88	0.41
4:Q:126:PHE:CZ	5:R:126:GLN:HG3	2.55	0.41
1:D:369:TYR:OH	1:D:388:ASN:ND2	2.52	0.41
1:D:502:GLY:O	1:D:506:GLN:HG3	2.21	0.41
1:C:486:PHE:HE2	4:X:2:VAL:HG21	1.85	0.41
1:A:337:PRO:HD2	1:A:358:ILE:HG23	2.03	0.41
1:A:369:TYR:OH	1:A:388:ASN:ND2	2.52	0.41
3:N:33:LEU:HD23	3:N:71:PHE:CG	2.55	0.41
1:D:405:ASP:OD1	5:T:94:TYR:CD2	2.73	0.41
1:D:460:ASN:OD1	4:S:54:GLY:CA	2.55	0.41
1:B:337:PRO:HD2	1:B:358:ILE:HG23	2.03	0.41
1:C:337:PRO:HD2	1:C:358:ILE:HG23	2.03	0.41
1:B:502:GLY:O	1:B:506:GLN:HG3	2.21	0.41
1:C:405:ASP:OD1	5:Y:94:TYR:CD2	2.74	0.41
2:E:194:THR:HG21	3:F:137:ASN:ND2	2.36	0.41
2:M:32:TYR:HB2	2:M:34:TRP:CZ2	2.56	0.41
2:J:32:TYR:HB2	2:J:34:TRP:CZ2	2.56	0.41
2:J:121:THR:HG21	2:J:158:PRO:CG	2.50	0.41
1:D:337:PRO:HD2	1:D:358:ILE:HG23	2.03	0.41
2:J:121:THR:CG2	2:J:158:PRO:HG3	2.51	0.41
1:C:455:LEU:O	4:X:33:TYR:OH	2.29	0.40
4:X:11:LEU:HD21	4:X:150:PHE:HE2	1.81	0.40
4:X:170:PHE:CD2	5:Y:166:THR:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:126:PHE:CD2	5:P:126:GLN:HG3	2.51	0.40
2:H:11:LEU:HB2	2:H:158:PRO:HG3	2.03	0.40
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.40
5:T:32:TYR:HB3	5:T:92:ASP:HB2	2.03	0.40
5:P:32:TYR:HB3	5:P:92:ASP:HB2	2.03	0.40
1:D:493:ARG:HD2	4:S:101:VAL:HG21	2.04	0.40
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.40
5:R:32:TYR:HB3	5:R:92:ASP:HB2	2.03	0.40
2:H:32:TYR:HB2	2:H:34:TRP:CZ2	2.56	0.40
1:C:487:ASN:HD21	4:X:27:VAL:HG22	1.87	0.40
5:Y:32:TYR:HB3	5:Y:92:ASP:HB2	2.03	0.40
5:P:108:ILE:HB	5:P:168:GLN:NE2	2.36	0.40
1:C:505:HIS:NE2	5:Y:29:ILE:HA	2.37	0.40
2:E:140:LYS:HB3	3:F:117:ILE:HG23	2.02	0.40
5:P:96:PRO:O	5:P:98:TYR:N	2.51	0.40
5:P:204:SER:HB2	4:Q:212:ASP:CB	2.51	0.40

All (4) 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)
3:F:188:LYS:O	2:H:217:LYS:N[1_565]	1.99	0.21
3:K:204:PRO:CG	4:Q:65:GLY:O[1_554]	2.10	0.10
5:T:190:LYS:NZ	2:H:103:VAL:O[1_655]	2.10	0.10
3:K:202:SER:OG	4:Q:57:THR:OG1[1_554]	2.19	0.01

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	193/202 (96%)	179 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	192/202 (95%)	178 (93%)	14 (7%)	0	100	100
1	C	193/202 (96%)	179 (93%)	14 (7%)	0	100	100
1	D	193/202 (96%)	179 (93%)	14 (7%)	0	100	100
2	E	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	17	56
2	H	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	17	56
2	J	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	17	56
2	M	220/229 (96%)	209 (95%)	9 (4%)	2 (1%)	17	56
3	F	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
3	K	207/214 (97%)	201 (97%)	6 (3%)	0	100	100
3	L	207/214 (97%)	201 (97%)	6 (3%)	0	100	100
3	N	206/214 (96%)	199 (97%)	7 (3%)	0	100	100
4	O	208/222 (94%)	202 (97%)	6 (3%)	0	100	100
4	Q	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
4	S	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
4	X	209/222 (94%)	203 (97%)	6 (3%)	0	100	100
5	P	211/216 (98%)	200 (95%)	9 (4%)	2 (1%)	17	56
5	R	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	17	56
5	T	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	17	56
5	Y	214/216 (99%)	203 (95%)	9 (4%)	2 (1%)	17	56
All	All	4167/4332 (96%)	3974 (95%)	177 (4%)	16 (0%)	34	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	109	ASP
2	M	109	ASP
5	Y	96	PRO
5	T	96	PRO
5	P	96	PRO
5	R	96	PRO
2	J	109	ASP
2	H	109	ASP
5	Y	97	GLY
5	T	97	GLY
5	P	97	GLY

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Mol	Chain	Res	Type
5	R	97	GLY
2	E	111	PHE
2	M	111	PHE
2	J	111	PHE
2	H	111	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/177 (95%)	167 (99%)	1 (1%)	86	92
1	B	167/177 (94%)	166 (99%)	1 (1%)	86	92
1	C	167/177 (94%)	166 (99%)	1 (1%)	86	92
1	D	168/177 (95%)	167 (99%)	1 (1%)	86	92
2	E	176/195 (90%)	173 (98%)	3 (2%)	60	78
2	H	178/195 (91%)	175 (98%)	3 (2%)	60	78
2	J	176/195 (90%)	173 (98%)	3 (2%)	60	78
2	M	178/195 (91%)	175 (98%)	3 (2%)	60	78
3	F	181/185 (98%)	179 (99%)	2 (1%)	73	85
3	K	178/185 (96%)	175 (98%)	3 (2%)	60	78
3	L	181/185 (98%)	178 (98%)	3 (2%)	60	78
3	N	177/185 (96%)	175 (99%)	2 (1%)	73	85
4	O	180/187 (96%)	180 (100%)	0	100	100
4	Q	181/187 (97%)	181 (100%)	0	100	100
4	S	181/187 (97%)	181 (100%)	0	100	100
4	X	181/187 (97%)	181 (100%)	0	100	100
5	P	187/188 (100%)	186 (100%)	1 (0%)	88	93
5	R	188/188 (100%)	187 (100%)	1 (0%)	88	93
5	T	187/188 (100%)	186 (100%)	1 (0%)	88	93
5	Y	188/188 (100%)	187 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3568/3728 (96%)	3538 (99%)	30 (1%)	81 89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	369	TYR
1	B	369	TYR
1	C	369	TYR
1	A	369	TYR
2	E	160	PRO
2	E	189	LEU
2	E	225	LYS
3	F	152	ASN
3	F	202	SER
3	K	152	ASN
3	K	165	GLU
3	K	202	SER
2	M	160	PRO
2	M	189	LEU
2	M	225	LYS
3	N	152	ASN
3	N	202	SER
3	L	108	ARG
3	L	152	ASN
3	L	202	SER
5	Y	91	LEU
5	T	91	LEU
5	P	91	LEU
5	R	91	LEU
2	J	160	PRO
2	J	189	LEU
2	J	225	LYS
2	H	160	PRO
2	H	189	LEU
2	H	225	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	477	ASN
2	E	39	GLN

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Mol	Chain	Res	Type
2	E	175	HIS
3	F	38	GLN
3	F	94	ASN
3	F	166	GLN
3	L	158	ASN
5	T	139	ASN
5	P	157	GLN
5	R	139	ASN
2	J	175	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.