



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:28 PM UTC

PDB ID : 3SCI / pdb_00003sci
Title : Crystal structure of spike protein receptor-binding domain from a predicted SARS coronavirus human strain complexed with human receptor ACE2
Authors : Wu, K.; Peng, G.; Wilken, M.; Geraghty, R.; Li, F.
Deposited on : 2011-06-07
Resolution : 2.90 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
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

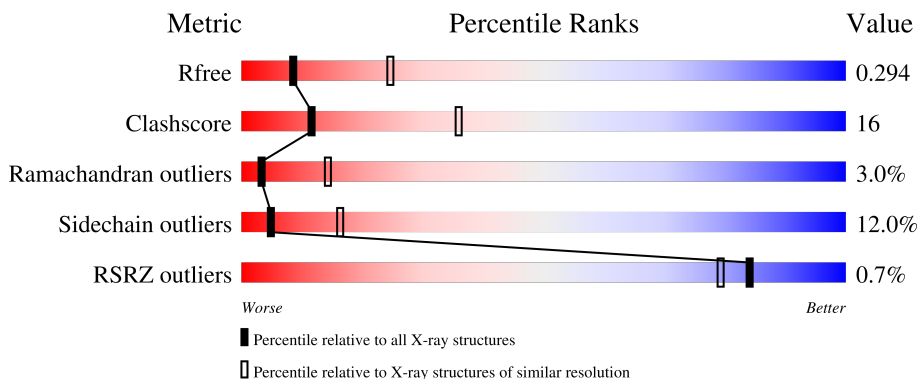
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	603	
1	B	603	
2	E	228	
2	F	228	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12552 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4870	3115	806	920	29	0	0	0
1	B	597	4870	3115	806	920	29	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
B	616	HIS	-	expression tag	UNP Q9BYF1
B	617	HIS	-	expression tag	UNP Q9BYF1
B	618	HIS	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	174	1404	912	228	257	7	0	0	0
2	F	174	1404	912	228	257	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	442	PHE	TYR	conflict	UNP P59594
E	472	PHE	LEU	conflict	UNP P59594
E	528	HIS	-	expression tag	UNP P59594
E	529	HIS	-	expression tag	UNP P59594
E	530	HIS	-	expression tag	UNP P59594
E	531	HIS	-	expression tag	UNP P59594
E	532	HIS	-	expression tag	UNP P59594
E	533	HIS	-	expression tag	UNP P59594
F	442	PHE	TYR	conflict	UNP P59594
F	472	PHE	LEU	conflict	UNP P59594
F	528	HIS	-	expression tag	UNP P59594
F	529	HIS	-	expression tag	UNP P59594
F	530	HIS	-	expression tag	UNP P59594
F	531	HIS	-	expression tag	UNP P59594
F	532	HIS	-	expression tag	UNP P59594
F	533	HIS	-	expression tag	UNP P59594

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

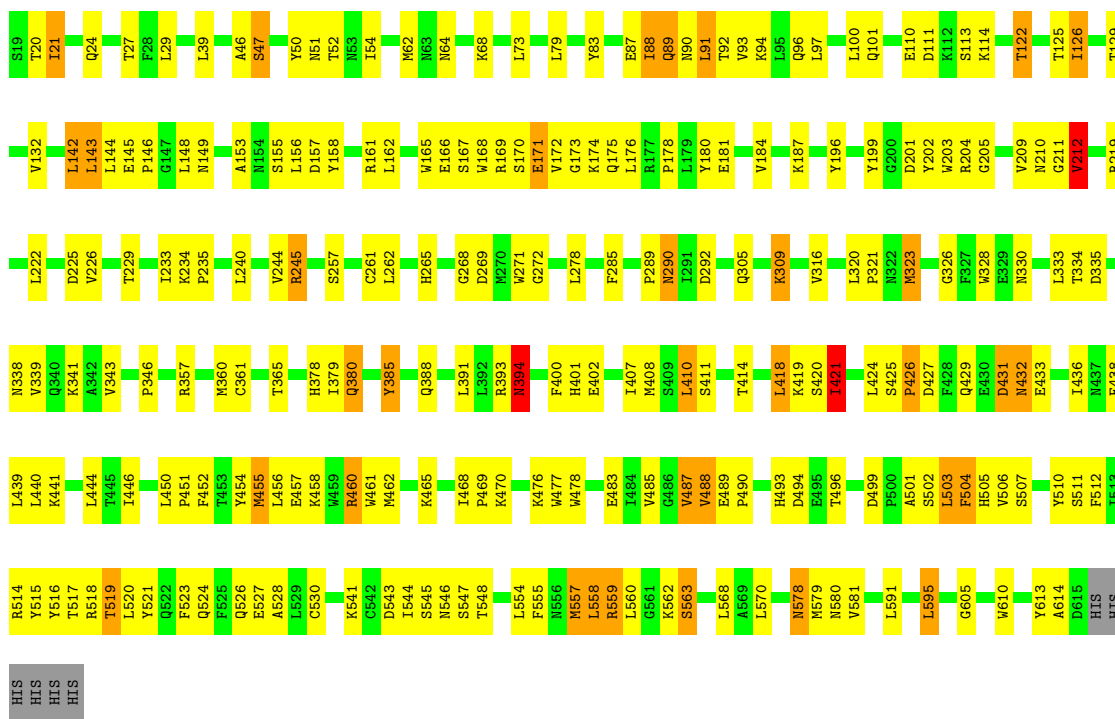
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

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.

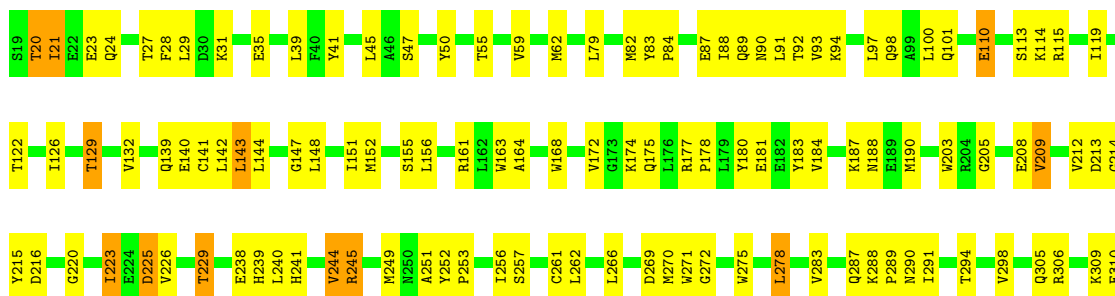
• Molecule 1: Angiotensin-converting enzyme 2

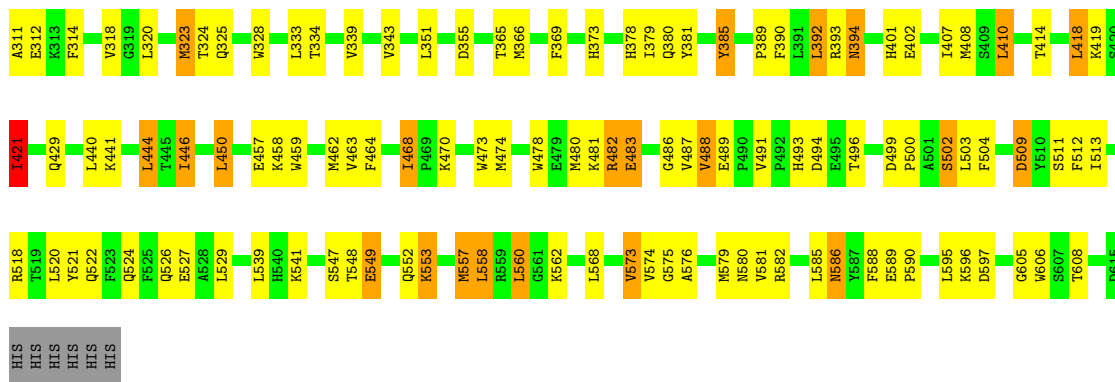
Chain A: 



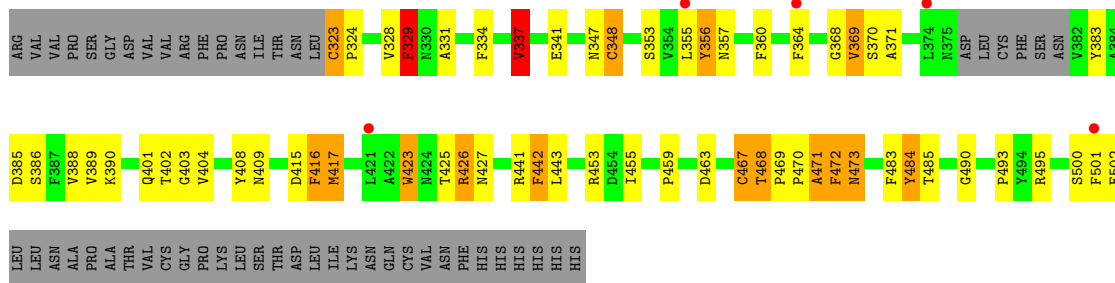
• Molecule 1: Angiotensin-converting enzyme 2

Chain B: 

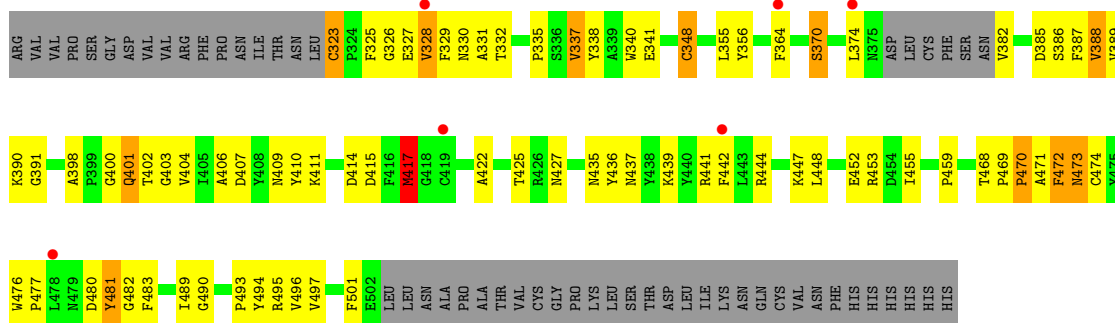




• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.36Å 118.33Å 111.94Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	47.24 – 2.90 47.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.5 (47.24-2.90) 84.9 (47.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.226 , 0.283 0.240 , 0.294	Depositor DCC
R_{free} test set	2270 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12552	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: ZN, CL

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	0.59	0/5007	0.92	3/6803 (0.0%)
1	B	0.61	0/5007	0.95	7/6803 (0.1%)
2	E	0.61	0/1450	0.93	5/1975 (0.3%)
2	F	0.59	0/1450	0.92	3/1975 (0.2%)
All	All	0.60	0/12914	0.93	18/17556 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	360	PHE	N-CA-C	-8.20	102.87	113.12
2	F	403	GLY	N-CA-C	7.08	120.11	110.69
1	B	257	SER	CA-C-N	6.77	128.31	119.84
1	B	257	SER	C-N-CA	6.77	128.31	119.84
1	B	225	ASP	N-CA-C	6.37	118.22	111.28
2	F	417	MET	N-CA-C	6.30	117.80	108.60
2	E	329	PHE	N-CA-C	-6.24	102.73	110.41
2	E	501	PHE	N-CA-C	6.16	118.89	107.99
1	B	468	ILE	CA-C-N	6.09	125.85	119.76
1	B	468	ILE	C-N-CA	6.09	125.85	119.76
1	B	547	SER	N-CA-C	5.71	118.01	107.73
1	B	214	GLY	N-CA-C	-5.70	108.18	115.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	403	GLY	N-CA-C	5.46	118.56	110.42
1	A	388	GLN	CA-C-N	-5.45	114.17	119.78
1	A	388	GLN	C-N-CA	-5.45	114.17	119.78
2	E	337	VAL	CB-CA-C	-5.43	104.81	112.14
1	A	563	SER	N-CA-C	5.31	116.87	111.14
2	F	398	ALA	N-CA-C	5.28	112.88	108.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ASN	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	A	4870	0	4643	155	0
1	B	4870	0	4643	152	0
2	E	1404	0	1325	38	0
2	F	1404	0	1325	46	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	12552	0	11936	391	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 (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:HE1	1:B:441:LYS:HE3	1.33	1.10
1:B:323:MET:HA	1:B:323:MET:HE3	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLN:HG3	1:B:83:TYR:HE2	1.29	0.95
2:E:409:ASN:HD21	2:E:441:ARG:H	1.15	0.95
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.47	0.94
1:B:245:ARG:HG2	1:B:245:ARG:HH21	1.34	0.91
1:B:393:ARG:O	1:B:394:ASN:HB2	1.73	0.89
1:B:407:ILE:HB	1:B:408:MET:HE2	1.54	0.86
1:A:122:THR:O	1:A:126:ILE:HG22	1.80	0.82
1:A:245:ARG:HH21	1:A:245:ARG:HG2	1.45	0.81
1:A:323:MET:HE3	1:A:323:MET:HA	1.61	0.81
1:A:407:ILE:HB	1:A:408:MET:HE2	1.63	0.79
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.66	0.76
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.23	0.74
2:E:472:PHE:O	2:E:473:ASN:HB2	1.88	0.74
2:E:453:ARG:NH1	2:E:455:ILE:HD11	2.04	0.72
1:A:455:MET:HE1	1:A:477:TRP:CZ3	2.24	0.72
1:B:549:GLU:CD	1:B:549:GLU:H	1.97	0.72
1:A:229:THR:HG23	1:A:516:TYR:OH	1.90	0.71
2:F:425:THR:HG21	2:F:495:ARG:HG3	1.73	0.71
1:B:262:LEU:O	1:B:487:VAL:HG13	1.91	0.71
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.72	0.69
1:A:285:PHE:HE1	1:A:436:ILE:HG21	1.56	0.69
2:F:439:LYS:HE2	2:F:480:ASP:OD2	1.92	0.69
1:A:457:GLU:OE2	1:A:512:PHE:N	2.26	0.69
1:B:20:THR:HG23	1:B:23:GLU:HB2	1.75	0.69
1:B:245:ARG:NH1	1:B:605:GLY:O	2.27	0.68
1:A:560:LEU:O	1:A:563:SER:HB3	1.93	0.68
1:B:366:MET:CE	1:B:441:LYS:HE3	2.19	0.68
1:B:478:TRP:O	1:B:482:ARG:HB2	1.93	0.68
1:B:122:THR:O	1:B:126:ILE:HG22	1.94	0.67
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.76	0.67
1:B:407:ILE:HD11	1:B:522:GLN:HA	1.76	0.67
2:F:417:MET:HA	2:F:417:MET:HE2	1.77	0.67
1:B:580:ASN:HD21	1:B:582:ARG:CZ	2.08	0.67
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.30	0.67
2:E:409:ASN:ND2	2:E:441:ARG:H	1.91	0.67
1:A:450:LEU:HD21	1:A:519:THR:HG21	1.76	0.66
1:B:139:GLN:HG3	1:B:140:GLU:H	1.60	0.66
2:E:353:SER:HA	2:E:356:TYR:HB2	1.76	0.66
1:A:142:LEU:HD23	1:A:143:LEU:HD12	1.78	0.66
1:A:21:ILE:H	1:A:21:ILE:HD13	1.61	0.65
1:A:47:SER:HA	1:A:62:MET:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASP:O	1:A:219:ARG:HD2	1.96	0.64
1:A:271:TRP:CE2	1:A:503:LEU:HD23	2.32	0.64
1:A:511:SER:O	1:A:514:ARG:HD2	1.98	0.64
1:A:21:ILE:HA	1:A:24:GLN:HG2	1.80	0.63
1:A:494:ASP:OD2	1:A:496:THR:HG22	1.98	0.63
1:B:459:TRP:O	1:B:463:VAL:HG23	1.97	0.63
1:A:142:LEU:HD23	1:A:143:LEU:H	1.63	0.63
1:B:366:MET:HE1	1:B:441:LYS:CE	2.19	0.63
1:B:21:ILE:HA	1:B:24:GLN:HG2	1.81	0.63
1:B:418:LEU:O	1:B:421:ILE:HG22	1.99	0.63
1:B:440:LEU:HD13	1:B:440:LEU:C	2.23	0.63
2:F:444:ARG:HH12	2:F:447:LYS:C	2.07	0.62
1:B:24:GLN:HG3	1:B:83:TYR:CE2	2.22	0.62
1:B:323:MET:HA	1:B:323:MET:CE	2.23	0.62
2:E:337:VAL:HG22	2:E:388:VAL:O	1.99	0.62
1:A:485:VAL:HG12	1:A:487:VAL:HG13	1.82	0.62
2:E:459:PRO:HB2	2:E:467:CYS:CB	2.30	0.61
1:B:245:ARG:HG2	1:B:245:ARG:NH2	2.10	0.61
1:B:351:LEU:HB2	1:B:355:ASP:HB3	1.81	0.61
1:A:271:TRP:CD2	1:A:503:LEU:HD23	2.35	0.61
1:A:126:ILE:HA	1:A:129:THR:HG22	1.84	0.60
1:A:514:ARG:HG2	1:A:515:TYR:N	2.16	0.60
1:A:438:PHE:O	1:A:441:LYS:HB3	2.01	0.60
1:B:249:MET:HG2	1:B:256:ILE:HB	1.83	0.60
1:A:378:HIS:CE1	1:A:402:GLU:OE1	2.55	0.60
2:F:472:PHE:O	2:F:473:ASN:HB2	2.01	0.60
1:B:90:ASN:O	1:B:92:THR:N	2.35	0.59
1:A:269:ASP:OD2	1:A:272:GLY:N	2.31	0.59
2:E:341:GLU:O	2:E:385:ASP:HA	2.02	0.59
2:E:364:PHE:HD2	2:E:364:PHE:O	1.86	0.59
1:A:499:ASP:O	1:A:502:SER:HB3	2.03	0.59
1:A:457:GLU:HG2	1:A:460:ARG:HH11	1.68	0.58
1:B:520:LEU:HD22	1:B:579:MET:CE	2.33	0.58
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.85	0.58
1:A:168:TRP:CD1	1:A:502:SER:HG	2.21	0.58
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.85	0.58
1:A:460:ARG:NE	1:A:506:VAL:HG22	2.18	0.58
1:A:514:ARG:HG2	1:A:515:TYR:H	1.68	0.58
1:B:275:TRP:HB3	1:B:278:LEU:HD22	1.84	0.58
2:E:426:ARG:HD3	2:E:485:THR:O	2.04	0.58
2:F:390:LYS:HG2	2:F:490:GLY:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:469:PRO:HG3	2:F:476:TRP:CZ2	2.40	0.57
1:A:501:ALA:O	1:A:507:SER:HB3	2.04	0.57
1:A:460:ARG:NH2	1:A:510:TYR:O	2.37	0.57
1:B:305:GLN:O	1:B:309:LYS:HB2	2.05	0.57
1:B:407:ILE:CD1	1:B:522:GLN:HA	2.34	0.56
1:A:225:ASP:O	1:A:229:THR:HG22	2.05	0.56
1:A:394:ASN:HB3	1:A:562:LYS:HG3	1.88	0.56
1:B:226:VAL:O	1:B:229:THR:HG22	2.04	0.56
2:F:325:PHE:C	2:F:327:GLU:H	2.12	0.56
2:F:435:ASN:O	2:F:482:GLY:HA2	2.05	0.56
1:A:591:LEU:HG	1:A:595:LEU:CD2	2.34	0.56
1:B:155:SER:O	1:B:161:ARG:HD2	2.05	0.56
1:A:199:TYR:O	1:A:202:TYR:HB3	2.05	0.56
1:A:489:GLU:HG2	1:A:613:TYR:HE2	1.69	0.56
2:F:406:ALA:HA	2:F:410:TYR:O	2.05	0.56
1:B:509:ASP:OD1	1:B:509:ASP:C	2.49	0.56
1:B:47:SER:HA	1:B:62:MET:HG3	1.87	0.56
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.86	0.56
1:A:456:LEU:CD2	1:A:477:TRP:HH2	2.19	0.55
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.88	0.55
2:E:472:PHE:O	2:E:473:ASN:CB	2.54	0.55
2:F:471:ALA:O	2:F:473:ASN:N	2.39	0.55
2:E:409:ASN:HD21	2:E:441:ARG:N	1.95	0.55
1:B:483:GLU:HA	1:B:606:TRP:HE1	1.71	0.55
1:B:520:LEU:HD22	1:B:579:MET:HE3	1.88	0.55
1:A:524:GLN:CD	1:A:580:ASN:H	2.14	0.55
1:B:275:TRP:O	1:B:278:LEU:HB2	2.06	0.55
1:B:385:TYR:O	1:B:393:ARG:HG2	2.07	0.55
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.72	0.55
1:B:574:VAL:HG23	1:B:575:GLY:N	2.22	0.55
1:A:455:MET:HE1	1:A:477:TRP:CE3	2.41	0.55
2:E:390:LYS:HG2	2:E:490:GLY:O	2.07	0.54
1:B:132:VAL:O	1:B:141:CYS:HB3	2.07	0.54
1:A:456:LEU:HD22	1:A:477:TRP:HH2	1.71	0.54
2:E:484:TYR:CD1	2:E:484:TYR:N	2.75	0.54
1:A:555:PHE:HA	1:A:558:LEU:HB2	1.88	0.54
1:B:41:TYR:CE2	1:B:45:LEU:HD11	2.42	0.54
1:B:126:ILE:HD11	1:B:175:GLN:HB2	1.90	0.54
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.72	0.54
1:B:489:GLU:OE1	1:B:489:GLU:N	2.34	0.54
1:B:574:VAL:HG23	1:B:576:ALA:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLU:HG2	1:A:460:ARG:NH1	2.22	0.54
2:E:442:PHE:CE2	2:E:443:LEU:HG	2.43	0.53
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.91	0.53
1:B:446:ILE:HD12	1:B:522:GLN:HE22	1.73	0.53
1:B:574:VAL:HG23	1:B:575:GLY:H	1.73	0.53
2:F:409:ASN:HD21	2:F:441:ARG:H	1.55	0.53
1:B:225:ASP:O	1:B:229:THR:HB	2.08	0.53
1:B:381:TYR:CD2	1:B:558:LEU:HG	2.43	0.53
2:F:340:TRP:CD1	2:F:340:TRP:H	2.26	0.53
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.53
1:B:294:THR:HG23	1:B:365:THR:HA	1.91	0.53
1:A:346:PRO:HB3	1:A:360:MET:HG3	1.91	0.53
1:A:393:ARG:O	1:A:394:ASN:HB2	2.09	0.53
1:B:270:MET:HB3	1:B:271:TRP:CE3	2.44	0.53
1:A:285:PHE:CE1	1:A:436:ILE:HG21	2.41	0.53
1:A:457:GLU:HG3	1:A:512:PHE:HB3	1.90	0.53
1:A:555:PHE:O	1:A:559:ARG:HG2	2.08	0.53
1:B:366:MET:O	1:B:369:PHE:HB3	2.09	0.53
1:A:233:ILE:HD11	1:A:581:VAL:HG21	1.91	0.52
1:B:126:ILE:HA	1:B:129:THR:HG22	1.91	0.52
1:A:169:ARG:O	1:A:173:GLY:HA3	2.09	0.52
2:F:400:GLY:O	2:F:401:GLN:HB2	2.09	0.52
2:F:422:ALA:HA	2:F:495:ARG:O	2.10	0.52
1:B:480:MET:HA	1:B:483:GLU:OE2	2.09	0.52
1:A:24:GLN:HG3	1:A:83:TYR:HE2	1.73	0.52
1:B:152:MET:HG3	1:B:270:MET:HA	1.92	0.52
1:A:96:GLN:HE21	1:A:391:LEU:HB2	1.75	0.52
1:B:239:HIS:CE1	1:B:596:LYS:HA	2.45	0.51
1:A:90:ASN:O	1:A:92:THR:N	2.43	0.51
1:A:330:ASN:HB3	1:A:357:ARG:NE	2.25	0.51
1:B:389:PRO:O	1:B:390:PHE:C	2.54	0.51
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.63	0.51
2:F:388:VAL:CG2	2:F:495:ARG:HG2	2.41	0.51
1:A:454:TYR:OH	1:A:458:LYS:NZ	2.44	0.51
1:A:524:GLN:NE2	1:A:580:ASN:H	2.09	0.51
1:B:271:TRP:NE1	1:B:502:SER:O	2.32	0.51
1:A:418:LEU:HB3	1:A:424:LEU:HB2	1.93	0.51
1:A:455:MET:O	1:A:455:MET:HE2	2.11	0.51
1:A:316:VAL:HA	1:A:320:LEU:O	2.09	0.51
1:B:94:LYS:O	1:B:98:GLN:HB2	2.10	0.51
2:F:329:PHE:C	2:F:331:ALA:H	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:337:VAL:HG13	2:F:387:PHE:CD1	2.46	0.51
2:F:435:ASN:OD1	2:F:436:TYR:N	2.44	0.51
2:F:483:PHE:CD2	2:F:493:PRO:HD3	2.45	0.51
2:E:388:VAL:CG2	2:E:495:ARG:HG2	2.41	0.50
1:B:294:THR:O	1:B:298:VAL:HG23	2.12	0.50
1:B:446:ILE:CD1	1:B:522:GLN:HE22	2.24	0.50
2:F:323:CYS:N	2:F:348:CYS:SG	2.84	0.50
1:A:503:LEU:O	1:A:504:PHE:C	2.54	0.50
1:A:142:LEU:HD22	1:A:146:PRO:O	2.12	0.50
1:A:450:LEU:HD21	1:A:519:THR:CG2	2.41	0.50
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.93	0.49
2:E:329:PHE:C	2:E:331:ALA:H	2.21	0.49
1:A:50:TYR:C	1:A:52:THR:H	2.20	0.49
1:A:411:SER:OG	1:A:544:ILE:HG12	2.12	0.49
1:B:318:VAL:O	1:B:548:THR:HA	2.13	0.49
1:A:97:LEU:O	1:A:101:GLN:HG2	2.13	0.49
1:A:468:ILE:HD12	1:A:476:LYS:HG3	1.94	0.49
1:A:153:ALA:HA	1:A:268:GLY:O	2.14	0.48
1:A:517:THR:O	1:A:518:ARG:C	2.56	0.48
1:A:526:GLN:O	1:A:530:CYS:SG	2.71	0.48
1:B:288:LYS:HB3	1:B:289:PRO:CD	2.43	0.48
2:E:337:VAL:HG21	2:E:389:VAL:HG12	1.94	0.48
2:F:327:GLU:O	2:F:331:ALA:HB2	2.12	0.48
2:F:391:GLY:HA2	2:F:494:TYR:CD1	2.48	0.48
1:A:204:ARG:HD2	1:A:219:ARG:O	2.13	0.48
1:A:323:MET:HA	1:A:323:MET:CE	2.39	0.48
1:A:432:ASN:HD22	1:A:433:GLU:N	2.12	0.48
2:E:417:MET:HE2	2:E:417:MET:HA	1.94	0.48
1:A:175:GLN:O	1:A:178:PRO:HD2	2.13	0.48
1:B:275:TRP:HB3	1:B:278:LEU:CD2	2.43	0.48
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.95	0.48
2:F:453:ARG:CZ	2:F:455:ILE:HD11	2.44	0.48
1:A:265:HIS:ND1	1:A:490:PRO:HG3	2.28	0.48
1:B:526:GLN:O	1:B:527:GLU:C	2.55	0.48
2:F:472:PHE:O	2:F:473:ASN:CB	2.62	0.48
1:A:335:ASP:HB2	1:A:361:CYS:HB3	1.96	0.48
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.61	0.48
2:E:368:GLY:O	2:E:369:VAL:HG13	2.14	0.47
2:E:388:VAL:HG22	2:E:495:ARG:HG2	1.96	0.47
1:A:433:GLU:O	1:A:436:ILE:HG22	2.15	0.47
1:B:291:ILE:O	1:B:291:ILE:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:PHE:O	2:E:364:PHE:CD2	2.66	0.47
1:B:238:GLU:O	1:B:241:HIS:HB3	2.14	0.47
1:B:524:GLN:NE2	1:B:580:ASN:H	2.12	0.47
2:F:406:ALA:O	2:F:411:LYS:HD2	2.14	0.47
1:A:338:ASN:HA	1:A:341:LYS:HE3	1.97	0.47
1:B:143:LEU:O	1:B:148:LEU:HB2	2.15	0.47
1:B:312:GLU:HG3	1:B:323:MET:HG2	1.96	0.47
2:E:467:CYS:O	2:E:468:THR:HG23	2.14	0.47
2:F:341:GLU:O	2:F:385:ASP:HA	2.14	0.47
1:A:245:ARG:HG2	1:A:245:ARG:NH2	2.22	0.47
1:A:245:ARG:NH1	1:A:605:GLY:O	2.48	0.47
1:A:167:SER:O	1:A:171:GLU:HG2	2.15	0.47
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.95	0.47
1:A:233:ILE:HD11	1:A:581:VAL:CG2	2.44	0.47
1:A:338:ASN:O	1:A:339:VAL:HB	2.15	0.47
1:B:220:GLY:HA2	1:B:223:ILE:HD12	1.96	0.47
1:B:378:HIS:CE1	1:B:402:GLU:OE1	2.68	0.47
1:B:499:ASP:N	1:B:500:PRO:HD2	2.30	0.47
1:B:589:GLU:OE1	1:B:589:GLU:HA	2.15	0.47
1:A:88:ILE:HB	1:A:94:LYS:HE3	1.96	0.47
1:A:578:ASN:ND2	1:A:579:MET:H	2.13	0.47
1:B:115:ARG:O	1:B:119:ILE:HG12	2.14	0.47
1:B:474:MET:HE1	1:B:499:ASP:OD1	2.14	0.47
1:A:414:THR:OG1	1:A:543:ASP:HB2	2.15	0.47
1:B:369:PHE:O	1:B:373:HIS:HD2	1.98	0.47
1:B:407:ILE:HB	1:B:408:MET:CE	2.36	0.47
1:B:414:THR:O	1:B:418:LEU:HD22	2.14	0.47
1:A:527:GLU:O	1:A:528:ALA:C	2.57	0.46
1:A:47:SER:HA	1:A:62:MET:CG	2.44	0.46
1:B:474:MET:HE1	1:B:499:ASP:CG	2.40	0.46
1:A:554:LEU:HG	1:A:558:LEU:HD22	1.97	0.46
1:B:311:ALA:O	1:B:314:PHE:HB3	2.16	0.46
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.97	0.46
1:A:90:ASN:HD22	1:A:93:VAL:HG13	1.80	0.46
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.96	0.46
2:E:423:TRP:CD1	2:E:423:TRP:N	2.84	0.46
2:F:469:PRO:HA	2:F:470:PRO:HA	1.74	0.46
1:B:324:THR:O	1:B:325:GLN:C	2.58	0.46
1:A:125:THR:O	1:A:129:THR:N	2.43	0.46
1:A:305:GLN:O	1:A:309:LYS:HB2	2.15	0.46
1:B:306:ARG:O	1:B:310:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLY:O	1:A:330:ASN:HB2	2.16	0.46
1:A:545:SER:C	1:A:547:SER:H	2.24	0.46
1:B:269:ASP:OD2	1:B:272:GLY:N	2.49	0.46
2:E:383:TYR:HE1	2:E:502:GLU:HB3	1.81	0.46
1:A:257:SER:HB2	1:A:610:TRP:CE2	2.50	0.46
1:B:208:GLU:HG2	1:B:209:VAL:N	2.30	0.46
1:A:456:LEU:HD22	1:A:477:TRP:CH2	2.49	0.46
1:B:184:VAL:O	1:B:188:ASN:HB2	2.16	0.45
1:B:97:LEU:O	1:B:101:GLN:HG2	2.16	0.45
1:A:245:ARG:HB2	1:A:262:LEU:HD21	1.97	0.45
1:B:249:MET:CG	1:B:256:ILE:HB	2.46	0.45
1:B:482:ARG:O	1:B:486:GLY:HA2	2.17	0.45
1:B:521:TYR:O	1:B:522:GLN:C	2.60	0.45
2:E:334:PHE:CE2	2:E:386:SER:HB2	2.51	0.45
1:A:516:TYR:O	1:A:519:THR:HG22	2.17	0.45
1:A:520:LEU:O	1:A:521:TYR:C	2.60	0.45
1:B:188:ASN:HD21	1:B:464:PHE:HA	1.82	0.45
2:E:471:ALA:O	2:E:472:PHE:C	2.60	0.45
1:B:504:PHE:C	1:B:504:PHE:CD2	2.94	0.45
1:A:187:LYS:HG2	1:A:199:TYR:CE2	2.52	0.44
1:A:462:MET:HE2	1:A:468:ILE:HD11	1.99	0.44
1:A:545:SER:O	1:A:547:SER:N	2.50	0.44
1:A:201:ASP:CG	1:A:219:ARG:HE	2.26	0.44
1:B:213:ASP:C	1:B:215:TYR:H	2.24	0.44
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.81	0.44
2:F:385:ASP:O	2:F:497:VAL:HA	2.17	0.44
2:F:388:VAL:HG22	2:F:495:ARG:HA	2.00	0.44
2:F:404:VAL:H	2:F:407:ASP:HB2	1.83	0.44
1:A:456:LEU:C	1:A:456:LEU:HD13	2.42	0.44
1:B:261:CYS:HB2	1:B:488:VAL:HG13	1.99	0.44
1:A:244:VAL:O	1:A:245:ARG:C	2.59	0.44
1:B:520:LEU:HD22	1:B:579:MET:HE1	1.99	0.44
2:F:325:PHE:C	2:F:327:GLU:N	2.73	0.44
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.53	0.44
1:B:240:LEU:O	1:B:244:VAL:HG13	2.18	0.44
1:B:526:GLN:HA	1:B:526:GLN:NE2	2.33	0.44
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.58	0.44
1:A:180:TYR:O	1:A:184:VAL:HG13	2.17	0.44
1:A:469:PRO:O	1:A:470:LYS:C	2.60	0.44
1:B:139:GLN:HG3	1:B:140:GLU:N	2.30	0.44
1:B:251:ALA:O	1:B:253:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:MET:HE1	1:B:379:ILE:CG2	2.48	0.44
2:E:469:PRO:HA	2:E:470:PRO:HA	1.74	0.44
2:F:471:ALA:O	2:F:474:CYS:N	2.42	0.44
1:B:440:LEU:CD1	1:B:444:LEU:HD22	2.47	0.43
1:B:503:LEU:HD23	1:B:504:PHE:N	2.32	0.43
1:B:553:LYS:HE3	1:B:573:VAL:HA	2.00	0.43
1:B:557:MET:HA	1:B:560:LEU:HD22	2.00	0.43
2:E:404:VAL:O	2:E:408:TYR:HB2	2.18	0.43
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.99	0.43
2:E:416:PHE:O	2:E:417:MET:CB	2.66	0.43
2:F:356:TYR:OH	2:F:370:SER:C	2.61	0.43
1:A:126:ILE:HG23	1:A:176:LEU:HD21	2.00	0.43
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.99	0.43
1:B:589:GLU:HB2	1:B:590:PRO:HD3	1.99	0.43
2:F:448:LEU:HD22	2:F:452:GLU:HG2	2.01	0.43
1:A:46:ALA:O	1:A:47:SER:C	2.62	0.43
1:A:203:TRP:C	1:A:205:GLY:N	2.74	0.43
1:B:183:TYR:O	1:B:187:LYS:HB2	2.19	0.43
1:B:494:ASP:OD2	1:B:494:ASP:N	2.47	0.43
1:B:147:GLY:O	1:B:151:ILE:HG12	2.19	0.43
1:B:275:TRP:N	1:B:275:TRP:CD1	2.84	0.43
1:A:88:ILE:HB	1:A:94:LYS:CE	2.48	0.43
1:A:424:LEU:HD12	1:A:424:LEU:HA	1.89	0.43
1:A:461:TRP:HB3	1:A:465:LYS:HE2	2.00	0.43
1:B:245:ARG:NH2	1:B:245:ARG:CG	2.81	0.43
1:B:499:ASP:O	1:B:500:PRO:C	2.61	0.43
2:E:337:VAL:CG2	2:E:389:VAL:HG12	2.49	0.43
1:A:68:LYS:HE3	1:A:68:LYS:HB2	1.69	0.43
1:A:385:TYR:C	1:A:385:TYR:CD2	2.97	0.43
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.48	0.43
1:A:290:ASN:HB3	1:A:292:ASP:HB3	2.01	0.42
1:B:110:GLU:OE2	1:B:110:GLU:HA	2.19	0.42
1:A:226:VAL:O	1:A:229:THR:HG22	2.19	0.42
1:A:514:ARG:CG	1:A:515:TYR:N	2.81	0.42
1:A:50:TYR:C	1:A:52:THR:N	2.78	0.42
1:B:93:VAL:HG23	1:B:94:LYS:N	2.34	0.42
2:F:389:VAL:HA	2:F:481:TYR:CE1	2.55	0.42
1:A:144:LEU:HA	1:A:148:LEU:HB2	2.00	0.42
1:A:400:PHE:CE2	1:A:557:MET:HE3	2.54	0.42
1:A:203:TRP:O	1:A:204:ARG:C	2.63	0.42
1:B:524:GLN:HB3	1:B:574:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASN:CG	1:B:581:VAL:H	2.28	0.42
1:B:552:GLN:O	1:B:553:LYS:C	2.62	0.42
2:F:386:SER:HA	2:F:496:VAL:O	2.20	0.42
1:A:145:GLU:HA	1:A:146:PRO:HA	1.87	0.42
1:A:196:TYR:CE2	1:A:202:TYR:HD2	2.38	0.42
1:B:168:TRP:CD1	1:B:502:SER:HB3	2.55	0.42
2:E:323:CYS:N	2:E:348:CYS:SG	2.93	0.42
1:A:111:ASP:C	1:A:113:SER:H	2.27	0.42
1:A:419:LYS:O	1:A:421:ILE:N	2.44	0.42
1:B:440:LEU:HD13	1:B:440:LEU:O	2.20	0.42
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.80	0.41
1:B:581:VAL:HG12	1:B:582:ARG:HH11	1.85	0.41
2:E:442:PHE:CD2	2:E:443:LEU:HG	2.55	0.41
1:A:89:GLN:HE21	1:A:89:GLN:HB3	1.66	0.41
1:B:50:TYR:CE1	1:B:59:VAL:HG23	2.55	0.41
1:B:203:TRP:C	1:B:205:GLY:N	2.75	0.41
1:B:457:GLU:HG3	1:B:513:ILE:N	2.35	0.41
1:B:526:GLN:HG3	1:B:539:LEU:HD11	2.02	0.41
2:F:356:TYR:HH	2:F:370:SER:C	2.27	0.41
1:A:157:ASP:O	1:A:158:TYR:C	2.63	0.41
1:A:493:HIS:HD2	1:A:499:ASP:OD2	2.03	0.41
1:B:31:LYS:O	1:B:35:GLU:HB2	2.20	0.41
1:B:163:TRP:O	1:B:164:ALA:C	2.63	0.41
1:B:177:ARG:HB3	1:B:178:PRO:HD3	2.01	0.41
1:B:389:PRO:HG2	1:B:392:LEU:HB2	2.01	0.41
2:F:459:PRO:HA	2:F:477:PRO:HD3	2.02	0.41
1:A:505:HIS:CD2	1:A:505:HIS:H	2.38	0.41
2:E:483:PHE:CD1	2:E:493:PRO:HB3	2.56	0.41
2:E:425:THR:HG21	2:E:495:ARG:HG3	2.01	0.41
2:F:328:VAL:O	2:F:331:ALA:HB3	2.21	0.41
1:A:211:GLY:O	1:A:212:VAL:C	2.64	0.41
1:B:83:TYR:HA	1:B:84:PRO:HD3	1.87	0.41
1:B:181:GLU:O	1:B:184:VAL:HG22	2.21	0.41
1:B:288:LYS:HB3	1:B:289:PRO:HD2	2.03	0.41
2:F:436:TYR:O	2:F:437:ASN:C	2.63	0.41
1:A:174:LYS:HG2	1:A:496:THR:O	2.20	0.41
1:A:431:ASP:C	1:A:433:GLU:N	2.79	0.41
2:F:382:VAL:HG22	2:F:501:PHE:CE2	2.56	0.41
1:A:170:SER:O	1:A:174:LYS:HG3	2.21	0.41
1:A:385:TYR:C	1:A:385:TYR:HD2	2.29	0.41
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PRO:O	1:B:290:ASN:C	2.63	0.41
2:E:484:TYR:N	2:E:484:TYR:HD1	2.17	0.41
1:A:425:SER:HA	1:A:426:PRO:HD2	1.89	0.40
1:A:455:MET:HE2	1:A:455:MET:C	2.46	0.40
2:F:329:PHE:O	2:F:330:ASN:HB2	2.22	0.40
1:A:410:LEU:HA	1:A:410:LEU:HD12	1.84	0.40
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.95	0.40
1:B:174:LYS:HA	1:B:496:THR:O	2.21	0.40
1:B:223:ILE:H	1:B:223:ILE:HG13	1.62	0.40
1:B:270:MET:HB3	1:B:271:TRP:CZ3	2.57	0.40
1:B:252:TYR:HD2	1:B:266:LEU:HD13	1.86	0.40
1:A:155:SER:O	1:A:161:ARG:HD2	2.22	0.40
1:B:586:ASN:C	1:B:588:PHE:N	2.76	0.40
2:F:337:VAL:HB	2:F:409:ASN:HD22	1.86	0.40
1:A:165:TRP:HZ2	1:A:478:TRP:HH2	1.70	0.40
1:A:261:CYS:HB2	1:A:488:VAL:HG13	2.03	0.40
1:A:451:PRO:O	1:A:452:PHE:C	2.65	0.40
1:B:187:LYS:O	1:B:190:MET:HB3	2.22	0.40
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.83	0.40
2:F:338:TYR:CE1	2:F:455:ILE:HG23	2.57	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	595/603 (99%)	506 (85%)	75 (13%)	14 (2%)	4	18
1	B	595/603 (99%)	516 (87%)	68 (11%)	11 (2%)	6	25
2	E	170/228 (75%)	131 (77%)	28 (16%)	11 (6%)	1	3
2	F	170/228 (75%)	135 (79%)	25 (15%)	10 (6%)	1	4
All	All	1530/1662 (92%)	1288 (84%)	196 (13%)	46 (3%)	3	14

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	212	VAL
1	B	91	LEU
1	B	394	ASN
1	B	421	ILE
2	E	402	THR
2	E	415	ASP
2	E	416	PHE
2	E	471	ALA
2	E	472	PHE
2	E	473	ASN
2	F	415	ASP
2	F	472	PHE
2	F	473	ASN
1	A	54	ILE
1	A	289	PRO
1	A	394	ASN
1	A	421	ILE
1	A	504	PHE
1	A	546	ASN
1	B	470	LYS
1	B	509	ASP
2	E	370	SER
2	E	371	ALA
2	F	374	LEU
1	A	420	SER
1	A	614	ALA
1	B	28	PHE
1	B	339	VAL
2	E	463	ASP
2	F	332	THR
2	F	401	GLN
1	A	51	ASN
1	A	64	ASN
1	A	171	GLU
1	B	113	SER
2	E	347	ASN
2	E	401	GLN
2	F	370	SER
2	F	402	THR
1	B	446	ILE
2	F	326	GLY

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Mol	Chain	Res	Type
1	B	89	GLN
1	A	426	PRO
1	B	212	VAL
2	F	470	PRO

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	527/533 (99%)	462 (88%)	65 (12%)	4	15
1	B	527/533 (99%)	461 (88%)	66 (12%)	4	15
2	E	152/202 (75%)	134 (88%)	18 (12%)	5	17
2	F	152/202 (75%)	138 (91%)	14 (9%)	8	27
All	All	1358/1470 (92%)	1195 (88%)	163 (12%)	5	16

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ILE
1	A	27	THR
1	A	29	LEU
1	A	39	LEU
1	A	47	SER
1	A	73	LEU
1	A	79	LEU
1	A	87	GLU
1	A	88	ILE
1	A	89	GLN
1	A	91	LEU
1	A	100	LEU
1	A	110	GLU
1	A	114	LYS
1	A	122	THR
1	A	126	ILE

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Mol	Chain	Res	Type
1	A	142	LEU
1	A	143	LEU
1	A	149	ASN
1	A	156	LEU
1	A	162	LEU
1	A	172	VAL
1	A	209	VAL
1	A	210	ASN
1	A	212	VAL
1	A	240	LEU
1	A	245	ARG
1	A	278	LEU
1	A	309	LYS
1	A	323	MET
1	A	333	LEU
1	A	334	THR
1	A	343	VAL
1	A	365	THR
1	A	380	GLN
1	A	385	TYR
1	A	394	ASN
1	A	401	HIS
1	A	410	LEU
1	A	418	LEU
1	A	421	ILE
1	A	427	ASP
1	A	429	GLN
1	A	431	ASP
1	A	432	ASN
1	A	439	LEU
1	A	440	LEU
1	A	444	LEU
1	A	455	MET
1	A	460	ARG
1	A	483	GLU
1	A	487	VAL
1	A	488	VAL
1	A	503	LEU
1	A	519	THR
1	A	541	LYS
1	A	548	THR
1	A	557	MET

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Mol	Chain	Res	Type
1	A	558	LEU
1	A	559	ARG
1	A	568	LEU
1	A	570	LEU
1	A	578	ASN
1	A	595	LEU
1	B	20	THR
1	B	21	ILE
1	B	27	THR
1	B	29	LEU
1	B	39	LEU
1	B	55	THR
1	B	79	LEU
1	B	82	MET
1	B	87	GLU
1	B	88	ILE
1	B	100	LEU
1	B	110	GLU
1	B	114	LYS
1	B	129	THR
1	B	142	LEU
1	B	143	LEU
1	B	156	LEU
1	B	172	VAL
1	B	209	VAL
1	B	216	ASP
1	B	223	ILE
1	B	229	THR
1	B	244	VAL
1	B	245	ARG
1	B	278	LEU
1	B	283	VAL
1	B	287	GLN
1	B	323	MET
1	B	333	LEU
1	B	334	THR
1	B	343	VAL
1	B	385	TYR
1	B	392	LEU
1	B	401	HIS
1	B	410	LEU
1	B	418	LEU

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Mol	Chain	Res	Type
1	B	419	LYS
1	B	421	ILE
1	B	429	GLN
1	B	444	LEU
1	B	450	LEU
1	B	458	LYS
1	B	462	MET
1	B	481	LYS
1	B	482	ARG
1	B	483	GLU
1	B	488	VAL
1	B	491	VAL
1	B	502	SER
1	B	511	SER
1	B	518	ARG
1	B	529	LEU
1	B	541	LYS
1	B	549	GLU
1	B	553	LYS
1	B	557	MET
1	B	558	LEU
1	B	560	LEU
1	B	562	LYS
1	B	568	LEU
1	B	573	VAL
1	B	585	LEU
1	B	586	ASN
1	B	595	LEU
1	B	597	ASP
1	B	608	THR
2	E	323	CYS
2	E	328	VAL
2	E	329	PHE
2	E	337	VAL
2	E	348	CYS
2	E	355	LEU
2	E	356	TYR
2	E	357	ASN
2	E	369	VAL
2	E	417	MET
2	E	423	TRP
2	E	426	ARG

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Mol	Chain	Res	Type
2	E	427	ASN
2	E	442	PHE
2	E	467	CYS
2	E	468	THR
2	E	484	TYR
2	E	500	SER
2	F	323	CYS
2	F	328	VAL
2	F	337	VAL
2	F	348	CYS
2	F	355	LEU
2	F	364	PHE
2	F	388	VAL
2	F	414	ASP
2	F	417	MET
2	F	427	ASN
2	F	442	PHE
2	F	468	THR
2	F	481	TYR
2	F	489	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	49	ASN
1	A	53	ASN
1	A	63	ASN
1	A	81	GLN
1	A	89	GLN
1	A	90	ASN
1	A	96	GLN
1	A	149	ASN
1	A	194	ASN
1	A	373	HIS
1	A	394	ASN
1	A	429	GLN
1	A	432	ASN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	522	GLN

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Mol	Chain	Res	Type
1	A	540	HIS
1	A	578	ASN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	49	ASN
1	B	51	ASN
1	B	53	ASN
1	B	58	ASN
1	B	61	ASN
1	B	63	ASN
1	B	96	GLN
1	B	98	GLN
1	B	103	ASN
1	B	117	ASN
1	B	194	ASN
1	B	277	ASN
1	B	290	ASN
1	B	300	GLN
1	B	330	ASN
1	B	373	HIS
1	B	394	ASN
1	B	493	HIS
1	B	508	ASN
1	B	522	GLN
1	B	524	GLN
1	B	526	GLN
1	B	531	GLN
1	B	552	GLN
1	B	556	ASN
1	B	572	ASN
1	B	580	ASN
2	E	409	ASN
2	F	409	ASN
2	F	437	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	597/603 (99%)	-0.35	0 100 100	39, 70, 116, 136	0
1	B	597/603 (99%)	-0.31	0 100 100	38, 73, 119, 138	0
2	E	174/228 (76%)	0.07	5 (2%) 53 45	64, 86, 128, 137	0
2	F	174/228 (76%)	0.13	6 (3%) 48 39	64, 88, 129, 138	0
All	All	1542/1662 (92%)	-0.23	11 (0%) 84 79	38, 75, 124, 138	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	442	PHE	3.1
2	E	501	PHE	2.8
2	F	364	PHE	2.8
2	F	374	LEU	2.7
2	E	374	LEU	2.3
2	F	478	LEU	2.2
2	E	355	LEU	2.1
2	E	364	PHE	2.1
2	F	419	CYS	2.0
2	E	421	LEU	2.0
2	F	328	VAL	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 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
4	CL	B	902	1/1	0.88	0.21	107,107,107,107	0
4	CL	A	902	1/1	0.91	0.13	92,92,92,92	0
3	ZN	B	901	1/1	0.94	0.13	90,90,90,90	0
3	ZN	A	901	1/1	0.96	0.12	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.