



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:59 AM EDT

PDB ID : 3SCL
Title : Crystal structure of spike protein receptor-binding domain from SARS coronavirus epidemic strain complexed with human-civet chimeric receptor ACE2
Authors : Wu, K.; Peng, G.; Wilken, M.; Geraghty, R.; Li, F.
Deposited on : 2011-06-07
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

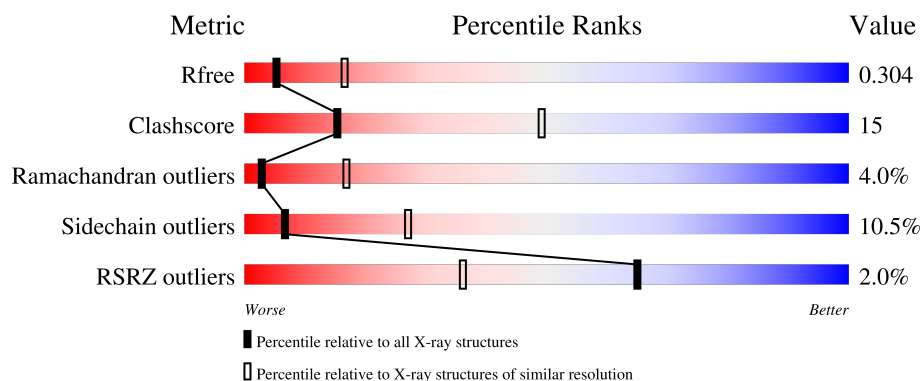
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>6%</div> <div>61% 32% 6%</div> </div>
1	B	603	<div> <div>59% 35%</div> </div>
2	E	185	<div> <div>3%</div> <div>55% 30% 8% 6%</div> </div>
2	F	185	<div> <div>6%</div> <div>62% 25% 5% 6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12522 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 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4863	3109	803	923	28			
1	B	597	Total	C	N	O	S	0	0	0
			4863	3109	803	923	28			

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
2	E	173	Total	C	N	O	S	0	0	0
			1396	906	227	257	6			
2	F	173	Total	C	N	O	S	0	0	0
			1396	906	227	257	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	503	HIS	-	expression tag	UNP P59594
E	504	HIS	-	expression tag	UNP P59594
E	505	HIS	-	expression tag	UNP P59594
E	506	HIS	-	expression tag	UNP P59594
E	507	HIS	-	expression tag	UNP P59594
E	508	HIS	-	expression tag	UNP P59594
F	503	HIS	-	expression tag	UNP P59594
F	504	HIS	-	expression tag	UNP P59594
F	505	HIS	-	expression tag	UNP P59594
F	506	HIS	-	expression tag	UNP P59594
F	507	HIS	-	expression tag	UNP P59594
F	508	HIS	-	expression tag	UNP P59594

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

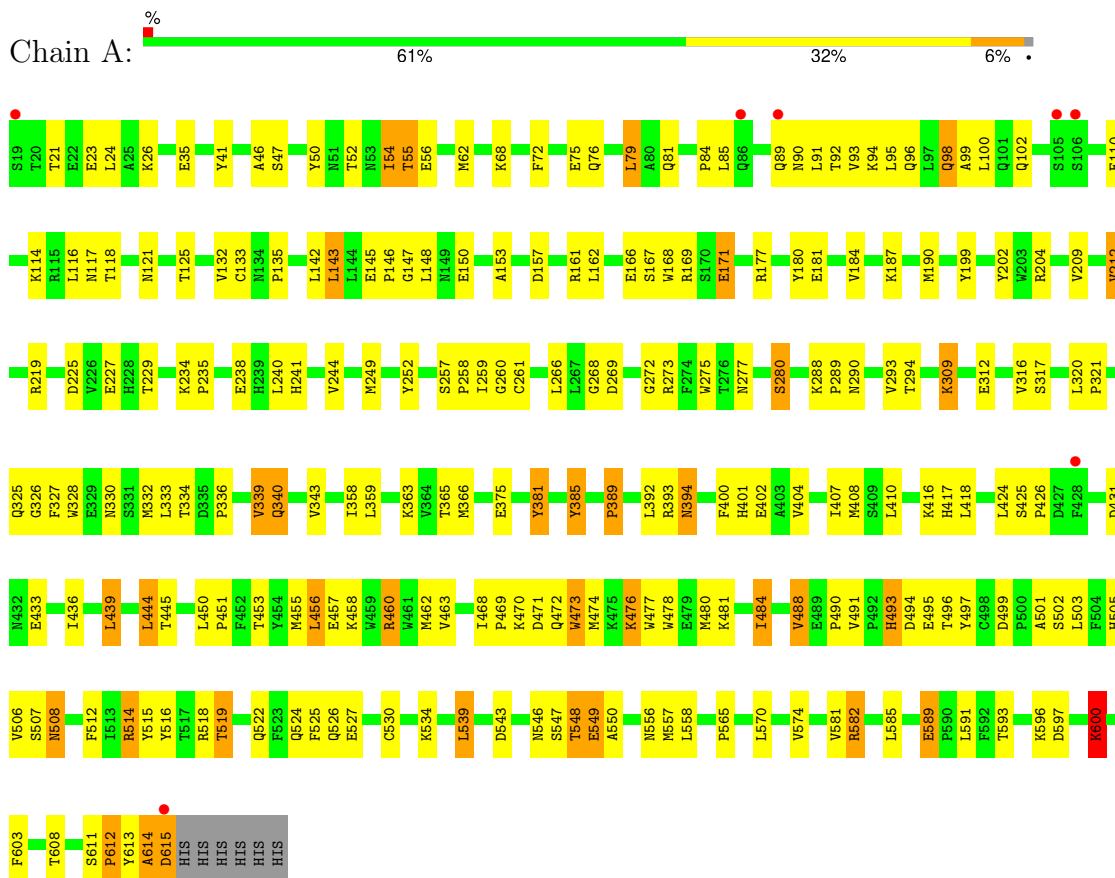
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

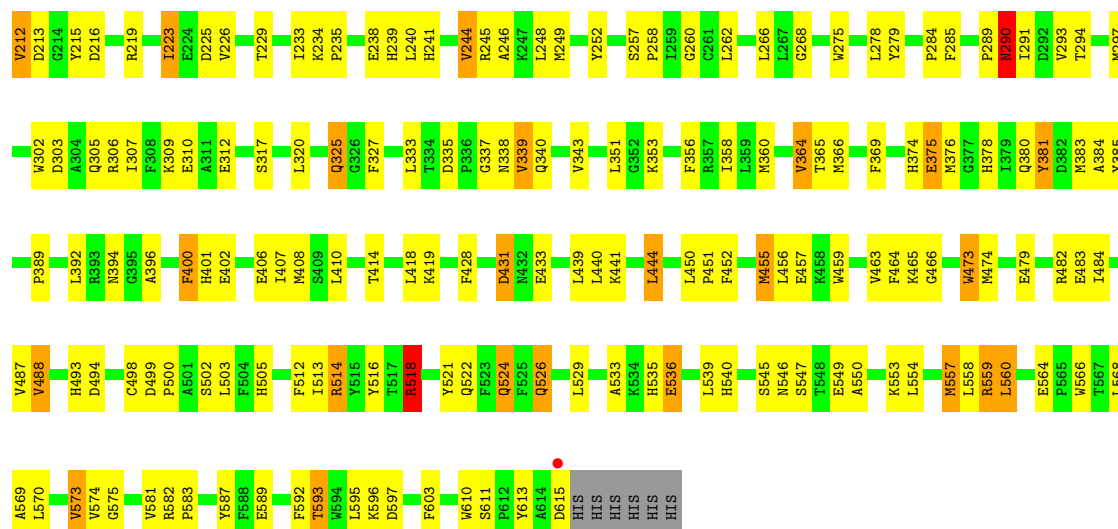
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0

3 Residue-property plots

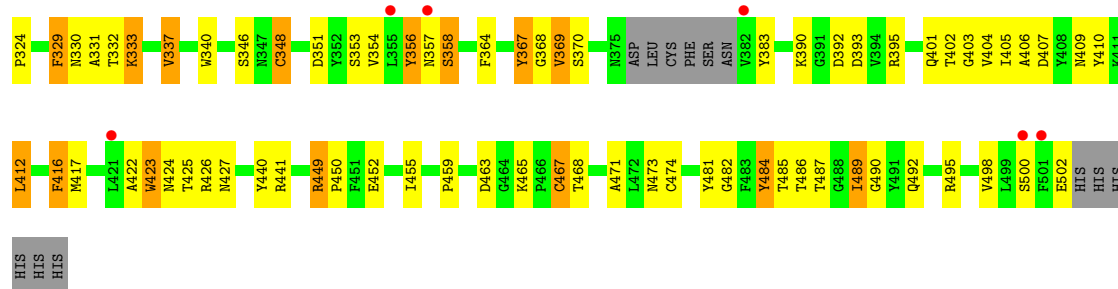
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

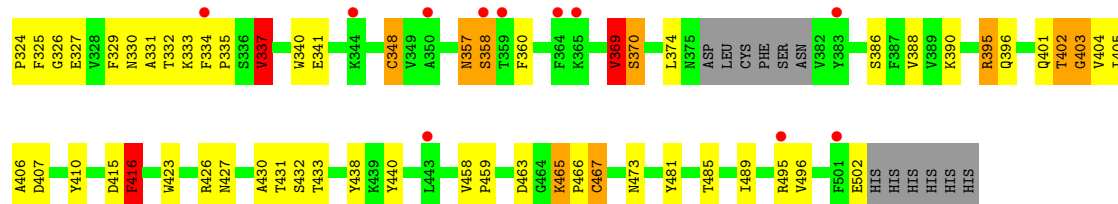




• Molecule 2: Spike glycoprotein



• 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	81.67Å 119.52Å 113.53Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	47.55 – 3.00 47.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.55-3.00) 94.6 (47.55-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.239 , 0.292 0.254 , 0.304	Depositor DCC
R_{free} test set	2170 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12522	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

5.1 Standard geometry

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	0/4999	0.69	0/6796
1	B	0.56	0/4999	0.67	2/6796 (0.0%)
2	E	0.62	0/1441	0.66	0/1963
2	F	0.56	0/1441	0.65	1/1963 (0.1%)
All	All	0.58	0/12880	0.67	3/17518 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	B	570	LEU	CA-CB-CG	5.72	128.46	115.30
2	F	403	GLY	N-CA-C	5.23	126.17	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4863	0	4636	141	0
1	B	4863	0	4636	152	0
2	E	1396	0	1325	41	0
2	F	1396	0	1325	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12522	0	11922	364	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 15.

All (364) 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)
2:F:324:PRO:HD2	2:F:348:CYS:SG	2.04	0.98
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.48	0.95
1:B:143:LEU:HD12	1:B:143:LEU:H	1.38	0.87
1:B:440:LEU:CD1	1:B:444:LEU:HD22	2.06	0.86
1:A:505:HIS:HE1	1:A:515:TYR:OH	1.59	0.85
1:B:99:ALA:O	1:B:102:GLN:HG3	1.77	0.84
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.62	0.81
1:A:229:THR:HG23	1:A:516:TYR:OH	1.82	0.80
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.66	0.77
1:A:416:LYS:HE2	1:A:543:ASP:HB3	1.67	0.77
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.67	0.77
1:B:249:MET:HE3	1:B:258:PRO:HA	1.66	0.77
1:A:474:MET:HE2	1:A:499:ASP:H	1.50	0.76
1:B:188:ASN:O	1:B:192:ARG:HG3	1.86	0.76
1:A:456:LEU:HD22	1:A:477:TRP:HH2	1.50	0.75
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.68	0.74
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.52	0.74
1:B:249:MET:HE3	1:B:258:PRO:CA	2.18	0.73
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.24	0.73
1:A:474:MET:CE	1:A:499:ASP:H	2.02	0.73
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.72	0.72
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.71	0.72
2:F:388:VAL:CG2	2:F:495:ARG:HG2	2.20	0.72
1:B:155:SER:O	1:B:161:ARG:NH1	2.23	0.71
2:E:357:ASN:O	2:E:358:SER:HB2	1.91	0.71
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.55	0.70
1:A:180:TYR:O	1:A:184:VAL:HG23	1.91	0.70
1:B:526:GLN:HG3	1:B:539:LEU:HD11	1.73	0.70
1:A:547:SER:HB3	1:A:550:ALA:HB3	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.46	0.69
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.74	0.68
1:B:24:LEU:HB2	1:B:83:TYR:HE2	1.58	0.67
1:B:306:ARG:O	1:B:310:GLU:HB2	1.96	0.66
1:B:226:VAL:O	1:B:229:THR:HG22	1.95	0.66
1:A:99:ALA:O	1:A:102:GLN:HG3	1.96	0.66
1:B:549:GLU:CD	1:B:549:GLU:H	1.98	0.66
1:A:600:LYS:HE3	1:A:600:LYS:HA	1.77	0.65
2:F:403:GLY:HA3	2:F:407:ASP:CG	2.17	0.65
1:A:162:LEU:HD13	1:A:490:PRO:HB2	1.78	0.65
1:B:414:THR:O	1:B:418:LEU:HD23	1.97	0.65
1:A:24:LEU:HD22	2:E:473:ASN:ND2	2.12	0.64
1:A:259:ILE:HG22	1:A:603:PHE:CD1	2.32	0.64
1:B:240:LEU:O	1:B:244:VAL:HG13	1.95	0.64
2:F:357:ASN:O	2:F:358:SER:HB2	1.98	0.64
1:B:339:VAL:O	1:B:340:GLN:HB3	1.96	0.64
1:B:406:GLU:O	1:B:410:LEU:HD13	1.98	0.63
1:B:402:GLU:HB3	1:B:518:ARG:HG3	1.80	0.63
2:E:424:ASN:OD1	2:E:426:ARG:HB2	1.98	0.63
1:A:143:LEU:HD12	1:A:143:LEU:H	1.65	0.62
1:B:529:LEU:HD11	1:B:554:LEU:HB2	1.80	0.62
1:A:90:ASN:O	1:A:92:THR:N	2.32	0.62
1:B:440:LEU:HD13	1:B:444:LEU:HD22	1.80	0.62
1:A:505:HIS:CE1	1:A:515:TYR:OH	2.48	0.62
1:B:440:LEU:HD11	1:B:444:LEU:HD22	1.81	0.62
1:A:199:TYR:O	1:A:202:TYR:HB3	2.00	0.61
2:F:325:PHE:C	2:F:327:GLU:H	2.03	0.61
1:A:407:ILE:HD11	1:A:525:PHE:HB2	1.82	0.61
1:A:293:VAL:HG22	1:A:366:MET:HG3	1.83	0.60
1:A:478:TRP:HA	1:A:481:LYS:HB2	1.83	0.60
1:B:209:VAL:HB	1:B:216:ASP:HA	1.82	0.60
2:E:455:ILE:HG22	2:E:455:ILE:O	2.02	0.60
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.83	0.60
1:A:457:GLU:OE2	1:A:460:ARG:NH1	2.35	0.60
1:A:519:THR:O	1:A:522:GLN:HG2	2.02	0.59
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.83	0.59
2:F:337:VAL:O	2:F:340:TRP:HD1	1.85	0.59
1:B:249:MET:HE3	1:B:258:PRO:N	2.18	0.59
1:A:417:HIS:HB2	1:A:543:ASP:OD2	2.03	0.58
1:A:52:THR:HB	1:A:332:MET:HE3	1.84	0.58
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:MET:HE2	1:B:499:ASP:H	1.68	0.58
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.85	0.57
1:A:153:ALA:HB1	1:A:277:ASN:OD1	2.04	0.57
1:B:294:THR:HG23	1:B:365:THR:HA	1.86	0.57
1:B:381:TYR:CE2	1:B:558:LEU:O	2.58	0.57
1:A:582:ARG:HB2	1:A:582:ARG:HH11	1.68	0.57
1:B:381:TYR:HE2	1:B:558:LEU:O	1.88	0.57
1:B:482:ARG:HE	1:B:488:VAL:HG12	1.69	0.57
2:E:329:PHE:H	2:E:329:PHE:HD2	1.53	0.57
1:A:225:ASP:O	1:A:229:THR:HG22	2.05	0.56
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.86	0.56
1:A:439:LEU:HB3	1:A:591:LEU:HD22	1.86	0.56
1:A:514:ARG:HG2	1:A:515:TYR:N	2.20	0.56
1:A:393:ARG:O	1:A:394:ASN:HB2	2.06	0.56
2:E:459:PRO:CB	2:E:467:CYS:HB3	2.36	0.56
2:F:327:GLU:O	2:F:331:ALA:HB2	2.05	0.56
2:E:406:ALA:HA	2:E:410:TYR:O	2.06	0.56
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.88	0.55
1:A:611:SER:HB2	1:A:614:ALA:HA	1.87	0.55
1:B:143:LEU:H	1:B:143:LEU:CD1	2.13	0.55
1:B:327:PHE:HE2	1:B:358:ILE:HG13	1.70	0.55
2:F:459:PRO:HB2	2:F:467:CYS:HB2	1.89	0.55
1:B:540:HIS:HA	1:B:587:TYR:CE1	2.42	0.55
2:E:405:ILE:HA	2:E:409:ASN:HD22	1.72	0.55
2:F:431:THR:C	2:F:433:THR:H	2.11	0.55
1:B:431:ASP:OD1	1:B:433:GLU:HB2	2.06	0.55
1:B:46:ALA:HB1	1:B:62:MET:HA	1.88	0.54
1:B:483:GLU:HB2	1:B:484:ILE:HG13	1.89	0.54
1:B:557:MET:HG2	1:B:573:VAL:HG21	1.90	0.54
2:F:403:GLY:C	2:F:405:ILE:H	2.10	0.54
1:A:460:ARG:NE	1:A:506:VAL:HG22	2.23	0.54
1:A:177:ARG:O	1:A:181:GLU:HG3	2.08	0.54
1:A:229:THR:OG1	1:A:581:VAL:HB	2.07	0.54
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.90	0.54
1:A:393:ARG:O	1:A:394:ASN:CB	2.56	0.54
1:A:453:THR:HG23	1:A:512:PHE:CD1	2.43	0.54
1:B:90:ASN:O	1:B:92:THR:N	2.41	0.53
1:B:535:HIS:CG	1:B:536:GLU:N	2.75	0.53
2:F:459:PRO:HB2	2:F:467:CYS:CB	2.38	0.53
1:B:559:ARG:HD2	1:B:560:LEU:HD13	1.89	0.53
1:B:49:ASN:O	1:B:53:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:422:ALA:C	2:E:423:TRP:HD1	2.12	0.53
1:A:326:GLY:O	1:A:330:ASN:HB2	2.08	0.53
1:B:302:TRP:O	1:B:364:VAL:HG21	2.08	0.53
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.90	0.53
2:E:329:PHE:C	2:E:331:ALA:H	2.11	0.53
1:B:366:MET:O	1:B:369:PHE:HB3	2.08	0.53
1:B:440:LEU:HD13	1:B:440:LEU:C	2.29	0.53
1:A:249:MET:HE1	1:A:258:PRO:HG3	1.90	0.53
1:A:407:ILE:HB	1:A:408:MET:HE2	1.91	0.53
1:B:47:SER:HA	1:B:62:MET:HG3	1.90	0.53
1:B:177:ARG:O	1:B:181:GLU:HG3	2.09	0.53
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.44	0.53
1:B:514:ARG:O	1:B:518:ARG:HB3	2.08	0.53
1:B:226:VAL:C	1:B:229:THR:HG22	2.29	0.52
1:A:55:THR:HG22	1:A:56:GLU:H	1.73	0.52
2:F:388:VAL:HG22	2:F:495:ARG:HG2	1.89	0.52
1:A:204:ARG:HD2	1:A:219:ARG:O	2.09	0.52
1:A:234:LYS:HB2	1:A:235:PRO:HD3	1.91	0.52
1:B:305:GLN:O	1:B:309:LYS:HB2	2.09	0.52
1:A:117:ASN:O	1:A:121:ASN:HB2	2.09	0.52
1:B:215:TYR:CE2	1:B:568:LEU:HD23	2.45	0.52
1:B:246:ALA:O	1:B:249:MET:HB2	2.08	0.52
1:A:229:THR:HG23	1:A:516:TYR:HH	1.73	0.52
2:E:383:TYR:HB2	2:E:500:SER:HB2	1.91	0.52
2:F:335:PRO:CG	2:F:341:GLU:HG2	2.38	0.52
1:A:494:ASP:OD2	1:A:496:THR:HG22	2.10	0.52
1:A:327:PHE:CE2	1:A:358:ILE:HG13	2.39	0.51
1:A:589:GLU:HA	1:A:589:GLU:OE1	2.09	0.51
1:B:293:VAL:HG11	1:B:418:LEU:HD12	1.92	0.51
1:B:239:HIS:CE1	1:B:596:LYS:HA	2.45	0.51
1:A:494:ASP:CG	1:A:496:THR:HG22	2.31	0.51
1:A:418:LEU:HB3	1:A:424:LEU:HB2	1.93	0.51
1:A:597:ASP:O	1:A:600:LYS:HB2	2.10	0.51
1:B:226:VAL:O	1:B:229:THR:CG2	2.58	0.51
1:A:339:VAL:O	1:A:340:GLN:CB	2.58	0.51
2:F:426:ARG:O	2:F:430:ALA:HB3	2.11	0.51
1:A:472:GLN:O	1:A:476:LYS:HB2	2.10	0.51
1:B:553:LYS:HE3	1:B:573:VAL:O	2.10	0.50
2:F:406:ALA:HA	2:F:410:TYR:O	2.11	0.50
1:B:146:PRO:O	1:B:150:GLU:HB2	2.12	0.50
1:B:257:SER:HB3	1:B:260:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.45	0.50
1:A:593:THR:HA	1:A:596:LYS:HE2	1.94	0.50
1:B:459:TRP:O	1:B:463:VAL:HG23	2.11	0.50
1:B:229:THR:HG23	1:B:516:TYR:OH	2.12	0.50
1:B:166:GLU:OE1	1:B:493:HIS:HE1	1.95	0.50
1:A:72:PHE:O	1:A:76:GLN:HG2	2.12	0.49
1:A:269:ASP:OD2	1:A:272:GLY:N	2.44	0.49
1:B:521:TYR:HA	1:B:524:GLN:HE21	1.77	0.49
1:B:94:LYS:O	1:B:98:GLN:HB2	2.12	0.49
1:B:333:LEU:O	1:B:360:MET:O	2.31	0.49
2:E:459:PRO:HB3	2:E:467:CYS:HB3	1.94	0.49
1:A:240:LEU:O	1:A:244:VAL:HG13	2.13	0.49
1:B:358:ILE:HD13	1:B:375:GLU:HB3	1.94	0.49
2:E:333:LYS:HD2	2:E:333:LYS:O	2.12	0.49
1:A:526:GLN:O	1:A:530:CYS:SG	2.71	0.48
2:F:369:VAL:HB	2:F:370:SER:H	1.48	0.48
1:A:259:ILE:HG22	1:A:603:PHE:HD1	1.77	0.48
1:B:63:ASN:O	1:B:67:ASP:N	2.45	0.48
2:E:484:TYR:CD1	2:E:484:TYR:N	2.81	0.48
1:A:252:TYR:CD2	1:A:266:LEU:HD13	2.48	0.48
1:A:309:LYS:HD2	1:A:328:TRP:CZ2	2.49	0.48
1:B:249:MET:CE	1:B:258:PRO:N	2.77	0.48
2:F:325:PHE:O	2:F:327:GLU:N	2.44	0.48
1:B:87:GLU:C	1:B:88:ILE:HG13	2.34	0.48
2:E:367:TYR:CD1	2:E:367:TYR:N	2.82	0.47
1:A:312:GLU:O	1:A:316:VAL:HG23	2.14	0.47
2:F:395:ARG:HH21	2:F:396:GLN:HG2	1.79	0.47
1:A:35:GLU:HB3	1:A:72:PHE:CZ	2.50	0.47
1:A:75:GLU:O	1:A:79:LEU:HB2	2.14	0.47
1:A:402:GLU:HB3	1:A:518:ARG:CD	2.43	0.47
1:B:499:ASP:O	1:B:500:PRO:C	2.52	0.47
2:E:404:VAL:H	2:E:407:ASP:HB2	1.79	0.47
1:A:209:VAL:HG11	1:A:565:PRO:HB3	1.95	0.47
1:A:227:GLU:OE2	1:A:458:LYS:HE2	2.15	0.47
2:F:440:TYR:CD1	2:F:440:TYR:C	2.88	0.47
1:B:81:GLN:C	1:B:83:TYR:H	2.18	0.47
1:B:223:ILE:H	1:B:223:ILE:HG13	1.45	0.47
1:B:275:TRP:HB2	1:B:444:LEU:HD12	1.96	0.47
2:E:424:ASN:ND2	2:E:492:GLN:OE1	2.38	0.47
1:A:46:ALA:HB1	1:A:62:MET:HA	1.96	0.47
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:O	1:B:291:ILE:HG22	2.14	0.47
1:B:574:VAL:HG23	1:B:575:GLY:N	2.29	0.47
1:A:508:ASN:N	1:A:508:ASN:HD22	2.12	0.47
1:A:288:LYS:HE2	1:A:433:GLU:HB2	1.95	0.47
1:B:327:PHE:CE2	1:B:358:ILE:HG13	2.49	0.47
2:E:422:ALA:C	2:E:423:TRP:CD1	2.88	0.47
1:A:294:THR:HG23	1:A:365:THR:HA	1.96	0.47
1:B:289:PRO:O	1:B:290:ASN:C	2.53	0.47
1:A:177:ARG:NH1	1:A:470:LYS:O	2.48	0.46
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.97	0.46
1:B:167:SER:O	1:B:171:GLU:HG2	2.15	0.46
1:B:238:GLU:O	1:B:241:HIS:HB3	2.15	0.46
1:A:468:ILE:HG12	1:A:476:LYS:HG3	1.96	0.46
1:B:166:GLU:OE1	1:B:493:HIS:CE1	2.68	0.46
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.51	0.46
1:B:239:HIS:NE2	1:B:596:LYS:HG2	2.29	0.46
1:B:374:HIS:NE2	1:B:378:HIS:NE2	2.62	0.46
1:B:521:TYR:HA	1:B:524:GLN:HB2	1.98	0.46
2:E:329:PHE:CD2	2:E:329:PHE:N	2.83	0.46
2:E:403:GLY:HA3	2:E:407:ASP:CG	2.36	0.46
1:B:582:ARG:HB3	1:B:583:PRO:HD3	1.96	0.46
2:E:484:TYR:HB2	2:E:487:THR:HG23	1.97	0.46
1:A:501:ALA:O	1:A:507:SER:HB3	2.16	0.46
1:B:414:THR:O	1:B:418:LEU:CD2	2.63	0.46
1:B:457:GLU:OE1	1:B:513:ILE:HB	2.15	0.46
1:B:566:TRP:HA	1:B:569:ALA:HB3	1.97	0.46
2:F:386:SER:HA	2:F:496:VAL:O	2.16	0.46
1:A:47:SER:HA	1:A:62:MET:HG3	1.97	0.46
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.80	0.46
1:B:384:ALA:HB1	1:B:559:ARG:HB3	1.97	0.46
1:B:589:GLU:O	1:B:593:THR:HG23	2.16	0.46
1:B:592:PHE:CE2	1:B:596:LYS:HE2	2.51	0.46
1:A:167:SER:O	1:A:171:GLU:HG2	2.16	0.46
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.67	0.46
1:B:505:HIS:H	1:B:505:HIS:CD2	2.32	0.46
2:E:440:TYR:CD1	2:E:440:TYR:C	2.89	0.46
1:B:574:VAL:HG23	1:B:575:GLY:H	1.81	0.45
1:A:157:ASP:O	1:A:161:ARG:HG3	2.15	0.45
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.52	0.45
1:B:535:HIS:CG	1:B:536:GLU:H	2.34	0.45
1:A:259:ILE:HG13	1:A:260:GLY:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:329:PHE:O	2:E:331:ALA:N	2.49	0.45
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.98	0.45
1:B:526:GLN:HA	1:B:526:GLN:NE2	2.26	0.45
2:F:426:ARG:HG2	2:F:485:THR:HG22	1.99	0.45
2:E:367:TYR:HD1	2:E:367:TYR:H	1.64	0.45
1:A:480:MET:O	1:A:484:ILE:HG12	2.16	0.45
1:A:505:HIS:CE1	1:A:515:TYR:CE2	3.05	0.45
2:E:449:ARG:HG3	2:E:452:GLU:OE1	2.17	0.45
1:B:431:ASP:OD1	1:B:433:GLU:N	2.41	0.45
1:A:410:LEU:HD23	1:A:526:GLN:HG3	1.98	0.45
1:B:143:LEU:O	1:B:144:LEU:C	2.54	0.45
1:B:440:LEU:CD1	1:B:444:LEU:CD2	2.88	0.45
2:E:337:VAL:O	2:E:340:TRP:HD1	2.00	0.45
1:B:21:THR:HG21	1:B:84:PRO:HD2	1.99	0.45
1:B:262:LEU:O	1:B:487:VAL:HA	2.16	0.45
1:B:278:LEU:O	1:B:279:TYR:C	2.56	0.45
1:B:521:TYR:O	1:B:522:GLN:C	2.54	0.45
2:F:324:PRO:CD	2:F:348:CYS:SG	2.92	0.45
1:A:257:SER:HA	1:A:258:PRO:HD3	1.86	0.44
1:A:547:SER:O	1:A:549:GLU:N	2.50	0.44
1:A:548:THR:HG22	1:A:549:GLU:N	2.32	0.44
1:B:177:ARG:HD2	1:B:498:CYS:SG	2.57	0.44
1:B:419:LYS:CD	1:B:428:PHE:HB3	2.48	0.44
2:E:324:PRO:CD	2:E:348:CYS:SG	3.06	0.44
1:A:145:GLU:HA	1:A:146:PRO:HA	1.66	0.44
1:B:245:ARG:NH1	1:B:603:PHE:O	2.50	0.44
1:B:407:ILE:HB	1:B:408:MET:HE2	1.99	0.44
1:B:533:ALA:HB2	1:B:550:ALA:HB2	2.00	0.44
2:E:409:ASN:OD1	2:E:441:ARG:N	2.38	0.44
1:A:549:GLU:H	1:A:549:GLU:HG3	1.54	0.44
1:B:109:SER:O	1:B:111:ASP:N	2.50	0.44
1:A:613:TYR:C	1:A:615:ASP:H	2.20	0.44
1:B:239:HIS:HB3	1:B:595:LEU:HB3	2.00	0.44
2:E:412:LEU:HD11	2:E:498:VAL:HG11	1.98	0.44
1:B:297:MET:CE	1:B:307:ILE:HD11	2.48	0.44
2:F:325:PHE:C	2:F:327:GLU:N	2.70	0.44
1:B:56:GLU:O	1:B:60:GLN:HG2	2.18	0.44
1:B:199:TYR:O	1:B:202:TYR:HB3	2.18	0.44
1:B:356:PHE:CE1	1:B:383:MET:HG2	2.53	0.44
1:A:275:TRP:O	1:A:444:LEU:HG	2.17	0.43
1:B:24:LEU:HB3	2:F:473:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD12	1:B:143:LEU:N	2.19	0.43
1:B:153:ALA:HA	1:B:268:GLY:O	2.18	0.43
1:B:234:LYS:HB2	1:B:235:PRO:HD3	2.00	0.43
2:F:337:VAL:O	2:F:340:TRP:CD1	2.68	0.43
1:A:181:GLU:OE1	1:A:470:LYS:HE3	2.17	0.43
1:A:570:LEU:HG	1:A:574:VAL:HG22	2.00	0.43
1:B:375:GLU:O	1:B:378:HIS:N	2.51	0.43
2:E:390:LYS:O	2:E:393:ASP:HB2	2.19	0.43
1:A:41:TYR:HH	2:E:486:THR:HG1	1.65	0.43
1:A:468:ILE:HA	1:A:469:PRO:HD3	1.84	0.43
2:F:458:VAL:HA	2:F:459:PRO:HD3	1.93	0.43
1:A:89:GLN:O	1:A:89:GLN:HG2	2.18	0.43
1:B:335:ASP:C	1:B:337:GLY:H	2.21	0.43
1:B:536:GLU:OE2	1:B:536:GLU:HA	2.17	0.43
2:E:346:SER:C	2:E:348:CYS:H	2.21	0.43
1:A:116:LEU:HD11	1:A:187:LYS:HD3	2.00	0.43
2:F:329:PHE:O	2:F:330:ASN:HB2	2.19	0.43
2:F:403:GLY:C	2:F:405:ILE:N	2.72	0.43
1:A:407:ILE:HD11	1:A:522:GLN:O	2.19	0.43
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.62	0.43
1:B:376:MET:O	1:B:376:MET:HG2	2.18	0.43
1:A:24:LEU:HB3	2:E:473:ASN:ND2	2.34	0.43
1:B:180:TYR:HA	1:B:183:TYR:HB3	2.01	0.43
1:B:457:GLU:C	1:B:459:TRP:H	2.23	0.43
1:B:464:PHE:C	1:B:466:GLY:H	2.22	0.43
1:A:23:GLU:OE1	1:A:26:LYS:HD2	2.19	0.42
1:B:198:ASP:OD1	1:B:465:LYS:HG2	2.19	0.42
1:A:381:TYR:CD2	1:A:558:LEU:HG	2.53	0.42
1:B:564:GLU:OE1	1:B:568:LEU:HD12	2.19	0.42
1:B:41:TYR:HD1	1:B:351:LEU:O	2.02	0.42
1:B:169:ARG:HB3	1:B:499:ASP:OD2	2.19	0.42
1:B:338:ASN:OD1	1:B:338:ASN:N	2.50	0.42
2:E:449:ARG:O	2:E:450:PRO:C	2.54	0.42
2:F:402:THR:O	2:F:407:ASP:OD1	2.36	0.42
1:A:68:LYS:HB3	1:A:68:LYS:HE2	1.87	0.42
1:B:248:LEU:HD12	1:B:262:LEU:HD22	2.01	0.42
2:F:465:LYS:HA	2:F:466:PRO:HD2	1.89	0.42
1:A:96:GLN:HG2	1:A:392:LEU:CD1	2.50	0.42
1:A:462:MET:O	1:A:463:VAL:C	2.56	0.42
1:B:457:GLU:HG2	1:B:512:PHE:HB3	2.01	0.42
1:B:284:PRO:HB2	1:B:285:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:MET:O	1:B:455:MET:CE	2.68	0.42
1:B:613:TYR:C	1:B:615:ASP:H	2.23	0.42
1:B:41:TYR:O	1:B:45:VAL:HG23	2.20	0.42
1:A:385:TYR:C	1:A:385:TYR:CD2	2.93	0.42
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.96	0.42
2:E:489:ILE:H	2:E:489:ILE:HG12	1.62	0.42
1:A:425:SER:HA	1:A:426:PRO:HD2	1.87	0.41
2:F:329:PHE:C	2:F:331:ALA:H	2.22	0.41
1:A:238:GLU:O	1:A:241:HIS:HB3	2.20	0.41
1:A:133:CYS:O	1:A:135:PRO:HD3	2.20	0.41
1:B:89:GLN:HG2	1:B:89:GLN:O	2.20	0.41
1:B:148:LEU:O	1:B:149:ASN:C	2.59	0.41
1:A:385:TYR:C	1:A:385:TYR:HD2	2.24	0.41
1:A:471:ASP:HA	1:A:495:GLU:HG3	2.02	0.41
1:B:545:SER:O	1:B:547:SER:N	2.53	0.41
1:A:145:GLU:OE2	1:A:146:PRO:HB3	2.20	0.41
1:A:153:ALA:HA	1:A:268:GLY:O	2.20	0.41
1:A:490:PRO:HA	1:A:612:PRO:HG2	2.02	0.41
1:B:257:SER:HA	1:B:258:PRO:HD3	1.92	0.41
1:B:312:GLU:HA	1:B:376:MET:SD	2.61	0.41
1:B:440:LEU:O	1:B:441:LYS:C	2.58	0.41
1:A:94:LYS:O	1:A:98:GLN:HB2	2.21	0.41
1:A:169:ARG:O	1:A:497:TYR:HD1	2.03	0.41
1:A:404:VAL:O	1:A:408:MET:HE2	2.21	0.41
1:B:325:GLN:HE21	1:B:325:GLN:HB3	1.63	0.41
1:A:527:GLU:HA	1:A:539:LEU:CD1	2.51	0.41
1:B:205:GLY:HA2	1:B:219:ARG:HD2	2.03	0.41
1:A:21:THR:HG21	1:A:84:PRO:HD2	2.02	0.41
1:A:249:MET:CE	1:A:258:PRO:HG3	2.51	0.41
1:B:479:GLU:O	1:B:483:GLU:HG2	2.21	0.41
2:E:471:ALA:O	2:E:474:CYS:HB2	2.20	0.41
2:F:388:VAL:HB	2:F:438:TYR:CE2	2.56	0.41
1:B:303:ASP:C	1:B:303:ASP:OD1	2.60	0.41
1:A:290:ASN:HD22	1:A:290:ASN:HA	1.69	0.40
1:B:28:PHE:HE2	1:B:76:GLN:OE1	2.04	0.40
1:A:252:TYR:HE2	1:A:266:LEU:HB3	1.86	0.40
1:A:332:MET:HE2	1:A:336:PRO:HG3	2.03	0.40
1:A:468:ILE:HG22	1:A:473:TRP:CD1	2.55	0.40
1:B:225:ASP:O	1:B:229:THR:HG22	2.21	0.40
1:B:440:LEU:CD1	1:B:440:LEU:C	2.89	0.40
2:E:392:ASP:OD1	2:E:490:GLY:HA2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:ILE:HD13	2:E:409:ASN:ND2	2.37	0.40
2:F:415:ASP:CG	2:F:416:PHE:H	2.24	0.40
1:A:468:ILE:CG2	1:A:473:TRP:HD1	2.33	0.40
1:B:396:ALA:HB3	1:B:400:PHE:CD2	2.57	0.40
2:E:351:ASP:C	2:E:353:SER:H	2.22	0.40
2:E:425:THR:HG21	2:E:495:ARG:HD2	2.03	0.40
1:B:514:ARG:HE	1:B:514:ARG:HB3	1.71	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%)	505 (85%)	73 (12%)	17 (3%)	4	24
1	B	595/603 (99%)	505 (85%)	71 (12%)	19 (3%)	4	22
2	E	169/185 (91%)	133 (79%)	24 (14%)	12 (7%)	1	5
2	F	169/185 (91%)	130 (77%)	26 (15%)	13 (8%)	1	5
All	All	1528/1576 (97%)	1273 (83%)	194 (13%)	61 (4%)	3	17

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	289	PRO
1	A	340	GLN
1	A	394	ASN
1	A	548	THR
1	B	91	LEU
2	E	358	SER
2	E	369	VAL

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Mol	Chain	Res	Type
2	E	401	GLN
2	F	369	VAL
2	F	402	THR
1	A	556	ASN
1	B	82	THR
1	B	110	GLU
1	B	212	VAL
1	B	353	LYS
2	E	402	THR
2	E	416	PHE
2	F	358	SER
2	F	374	LEU
2	F	390	LYS
2	F	404	VAL
2	F	416	PHE
1	A	534	LYS
1	A	600	LYS
1	B	85	LEU
1	B	171	GLU
1	B	290	ASN
1	B	546	ASN
2	E	330	ASN
2	E	463	ASP
2	E	465	LYS
2	F	337	VAL
2	F	370	SER
1	A	539	LEU
1	B	213	ASP
1	B	452	PHE
1	B	473	TRP
1	B	536	GLU
1	B	610	TRP
2	E	356	TYR
2	E	368	GLY
2	E	370	SER
2	F	401	GLN
2	F	432	SER
1	A	171	GLU
1	A	212	VAL
1	A	280	SER
1	A	546	ASN
1	A	614	ALA

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Mol	Chain	Res	Type
2	F	465	LYS
1	B	211	GLY
1	B	339	VAL
1	B	581	VAL
2	F	326	GLY
1	A	612	PRO
1	B	451	PRO
1	A	54	ILE
1	A	339	VAL
2	E	482	GLY
1	B	364	VAL

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	527/533 (99%)	471 (89%)	56 (11%)	6	26
1	B	527/533 (99%)	481 (91%)	46 (9%)	10	37
2	E	151/163 (93%)	127 (84%)	24 (16%)	2	12
2	F	151/163 (93%)	134 (89%)	17 (11%)	6	24
All	All	1356/1392 (97%)	1213 (90%)	143 (10%)	7	27

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	79	LEU
1	A	81	GLN
1	A	85	LEU
1	A	95	LEU
1	A	98	GLN
1	A	100	LEU
1	A	110	GLU
1	A	114	LYS
1	A	118	THR

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Mol	Chain	Res	Type
1	A	125	THR
1	A	143	LEU
1	A	148	LEU
1	A	150	GLU
1	A	190	MET
1	A	212	VAL
1	A	273	ARG
1	A	280	SER
1	A	309	LYS
1	A	317	SER
1	A	325	GLN
1	A	333	LEU
1	A	334	THR
1	A	343	VAL
1	A	363	LYS
1	A	375	GLU
1	A	381	TYR
1	A	385	TYR
1	A	389	PRO
1	A	400	PHE
1	A	401	HIS
1	A	431	ASP
1	A	439	LEU
1	A	444	LEU
1	A	445	THR
1	A	455	MET
1	A	456	LEU
1	A	460	ARG
1	A	473	TRP
1	A	476	LYS
1	A	484	ILE
1	A	488	VAL
1	A	491	VAL
1	A	493	HIS
1	A	503	LEU
1	A	508	ASN
1	A	514	ARG
1	A	519	THR
1	A	549	GLU
1	A	557	MET
1	A	582	ARG
1	A	585	LEU

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Mol	Chain	Res	Type
1	A	589	GLU
1	A	600	LYS
1	A	608	THR
1	A	615	ASP
1	B	55	THR
1	B	81	GLN
1	B	95	LEU
1	B	98	GLN
1	B	100	LEU
1	B	114	LYS
1	B	121	ASN
1	B	125	THR
1	B	139	GLN
1	B	143	LEU
1	B	187	LYS
1	B	190	MET
1	B	212	VAL
1	B	223	ILE
1	B	244	VAL
1	B	290	ASN
1	B	317	SER
1	B	325	GLN
1	B	343	VAL
1	B	375	GLU
1	B	381	TYR
1	B	385	TYR
1	B	394	ASN
1	B	400	PHE
1	B	401	HIS
1	B	431	ASP
1	B	439	LEU
1	B	444	LEU
1	B	455	MET
1	B	456	LEU
1	B	473	TRP
1	B	488	VAL
1	B	494	ASP
1	B	502	SER
1	B	503	LEU
1	B	514	ARG
1	B	518	ARG
1	B	524	GLN

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Mol	Chain	Res	Type
1	B	526	GLN
1	B	557	MET
1	B	559	ARG
1	B	560	LEU
1	B	573	VAL
1	B	593	THR
1	B	597	ASP
1	B	611	SER
2	E	329	PHE
2	E	332	THR
2	E	333	LYS
2	E	337	VAL
2	E	348	CYS
2	E	354	VAL
2	E	356	TYR
2	E	364	PHE
2	E	367	TYR
2	E	369	VAL
2	E	395	ARG
2	E	412	LEU
2	E	416	PHE
2	E	417	MET
2	E	423	TRP
2	E	427	ASN
2	E	449	ARG
2	E	467	CYS
2	E	468	THR
2	E	481	TYR
2	E	484	TYR
2	E	485	THR
2	E	489	ILE
2	E	502	GLU
2	F	332	THR
2	F	333	LYS
2	F	334	PHE
2	F	337	VAL
2	F	348	CYS
2	F	357	ASN
2	F	360	PHE
2	F	369	VAL
2	F	395	ARG
2	F	416	PHE

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Mol	Chain	Res	Type
2	F	423	TRP
2	F	427	ASN
2	F	463	ASP
2	F	467	CYS
2	F	481	TYR
2	F	489	ILE
2	F	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	GLN
1	A	64	ASN
1	A	81	GLN
1	A	90	ASN
1	A	103	ASN
1	A	139	GLN
1	A	149	ASN
1	A	221	GLN
1	A	290	ASN
1	A	300	GLN
1	A	394	ASN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	535	HIS
1	A	546	ASN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	53	ASN
1	B	96	GLN
1	B	102	GLN
1	B	103	ASN
1	B	139	GLN
1	B	154	ASN
1	B	194	ASN
1	B	221	GLN
1	B	250	ASN
1	B	277	ASN
1	B	290	ASN

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Mol	Chain	Res	Type
1	B	300	GLN
1	B	325	GLN
1	B	394	ASN
1	B	505	HIS
1	B	526	GLN
1	B	540	HIS
1	B	552	GLN
1	B	572	ASN
1	B	586	ASN
1	B	598	GLN
1	B	599	ASN
1	B	601	ASN
2	E	473	ASN
2	F	330	ASN
2	F	375	ASN
2	F	473	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

6.1 Protein, DNA and RNA chains

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%)	-0.17	7 (1%)	79 54	30, 69, 117, 140	0
1	B	597/603 (99%)	-0.13	7 (1%)	79 54	35, 70, 118, 141	0
2	E	173/185 (93%)	-0.01	6 (3%)	44 18	56, 84, 123, 130	0
2	F	173/185 (93%)	0.19	11 (6%)	19 6	60, 85, 123, 131	0
All	All	1540/1576 (97%)	-0.10	31 (2%)	65 36	30, 74, 120, 141	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	615	ASP	5.3
2	E	501	PHE	3.8
1	A	428	PHE	3.8
1	A	86	GLN	3.7
1	A	19	SER	3.5
2	E	382	VAL	3.2
1	A	89	GLN	3.1
1	B	136	ASP	2.9
2	F	350	ALA	2.9
2	F	501	PHE	2.8
2	E	421	LEU	2.8
1	B	105	SER	2.7
1	A	615	ASP	2.7
2	F	364	PHE	2.6
2	F	495	ARG	2.6
1	B	89	GLN	2.5
1	A	106	SER	2.5
2	F	383	TYR	2.4
2	E	357	ASN	2.4
1	B	129	THR	2.3
2	F	443	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	355	LEU	2.2
1	B	135	PRO	2.2
2	F	359	THR	2.2
2	F	365	LYS	2.2
2	F	358	SER	2.1
1	A	105	SER	2.1
2	F	334	PHE	2.1
2	E	500	SER	2.1
1	B	137	ASN	2.0
2	F	344	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZN	A	901	1/1	0.81	0.37	102,102,102,102	0
4	CL	A	902	1/1	0.83	0.55	104,104,104,104	0
3	ZN	B	901	1/1	0.94	0.48	102,102,102,102	0
4	CL	B	902	1/1	0.95	0.45	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.