Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID	:	3SCJ
Title	:	Crystal structure of spike protein receptor-binding domain from a predicted SARS coronavirus civet strain complexed with human 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
http://wwpdb.org/validation/2016/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:

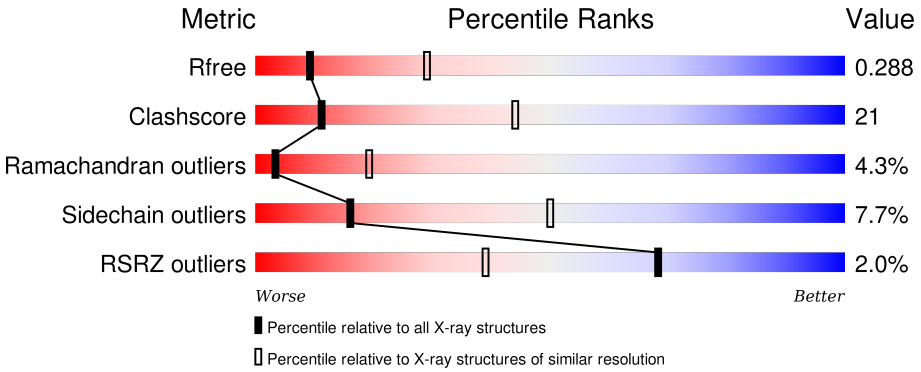
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	603	57% 36% 5%
1	B	603	2% 55% 38% 5%
2	E	186	4% 54% 32% 7% 6%
2	F	186	3% 58% 30% 6% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	902	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12544 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
1	A	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			
1	B	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			

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	174	Total	C	N	O	S	0	0	0
			1400	908	230	255	7			
2	F	174	Total	C	N	O	S	0	0	0
			1400	908	230	255	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	472	PRO	LEU	SEE REMARK 999	UNP P59594
E	479	ARG	ASN	CONFLICT	UNP P59594
E	480	GLY	ASP	SEE REMARK 999	UNP P59594
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	472	PRO	LEU	SEE REMARK 999	UNP P59594
F	479	ARG	ASN	CONFLICT	UNP P59594
F	480	GLY	ASP	SEE REMARK 999	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	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

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

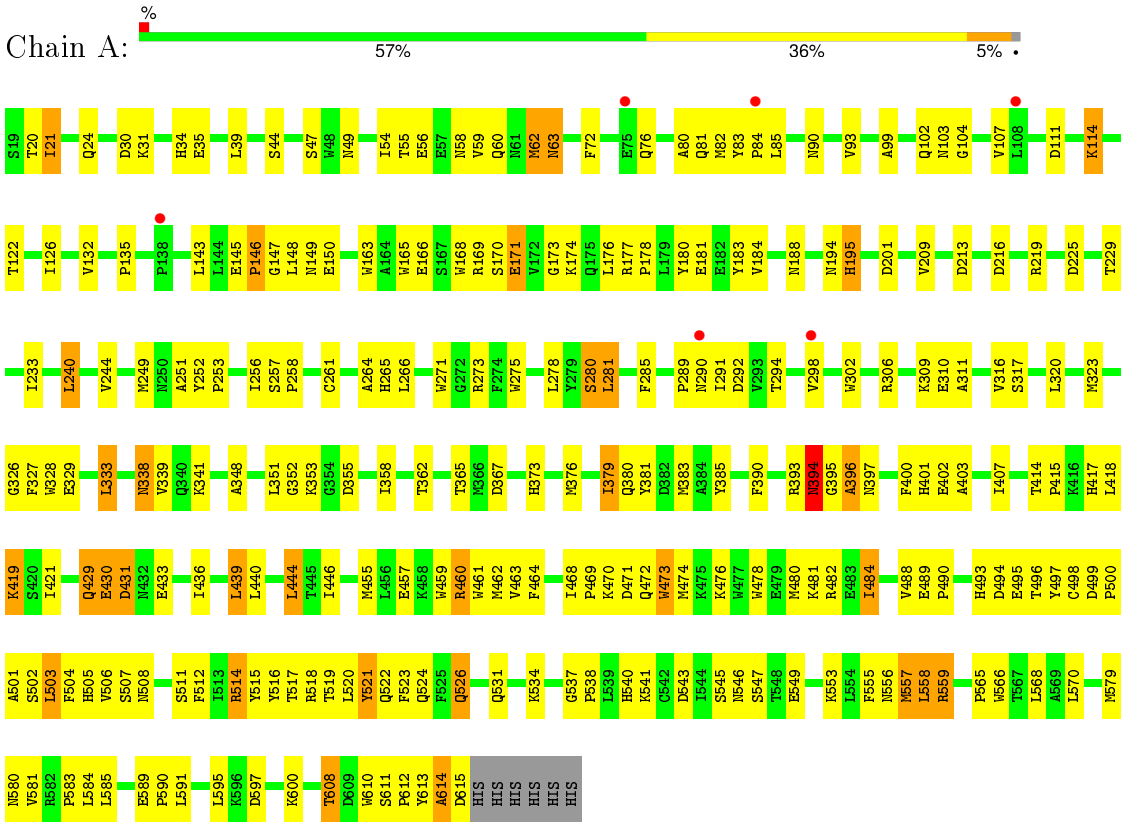
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

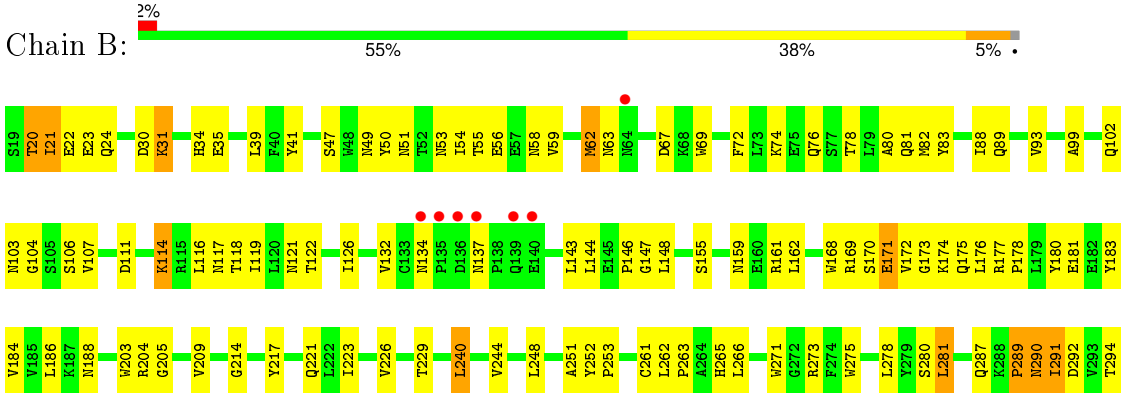
- Molecule 1: Angiotensin-converting enzyme 2

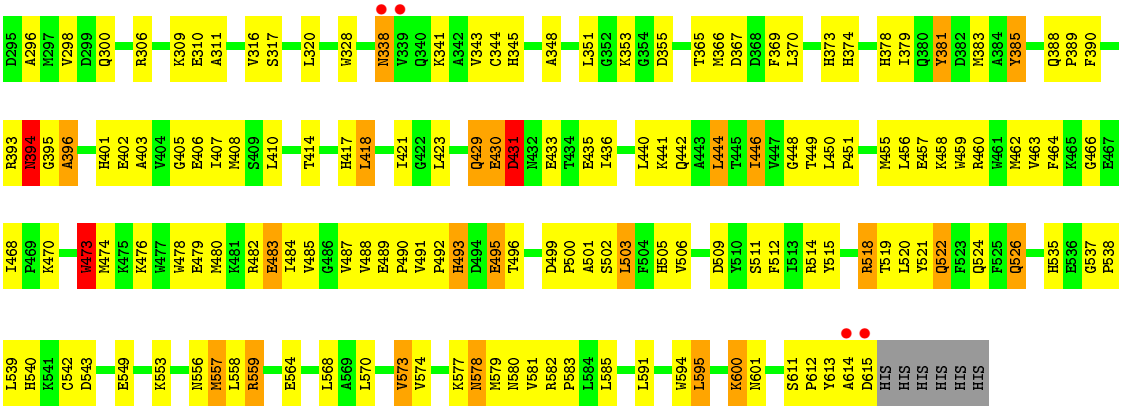
Chain A:



- Molecule 1: Angiotensin-converting enzyme 2

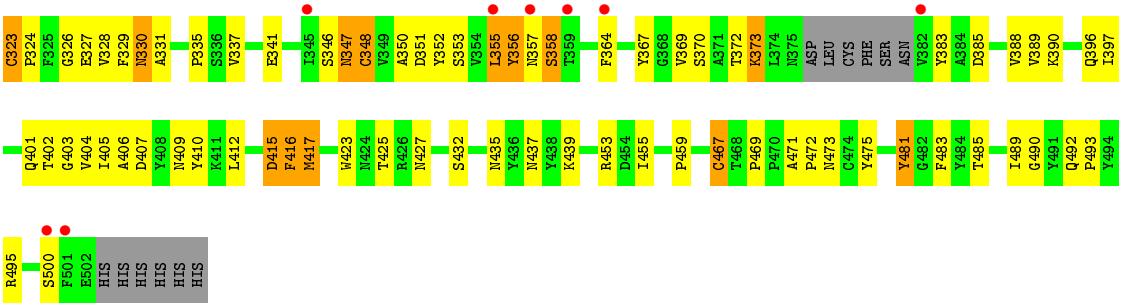
Chain B:





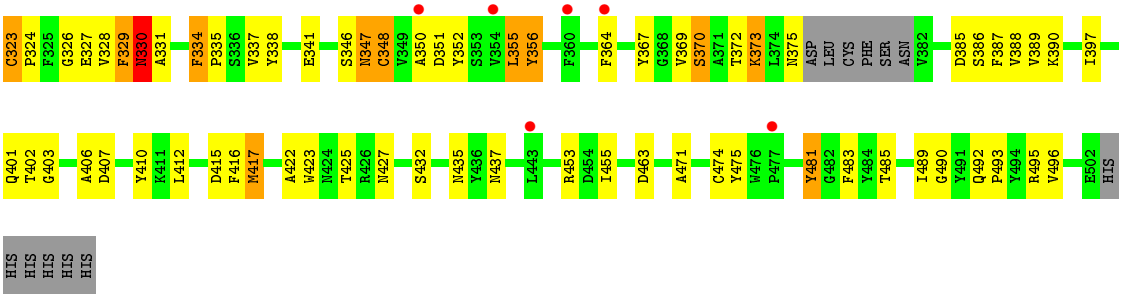
- Molecule 2: Spike glycoprotein

Chain E:



- Molecule 2: Spike glycoprotein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.22Å 119.28Å 113.24Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	47.27 – 3.00 47.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.3 (47.27-3.00) 87.2 (47.27-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.278 0.237 , 0.288	Depositor DCC
R_{free} test set	2153 reflections (6.01%)	DCC
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 30.2	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 43229 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12544	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/5007	0.61	0/6803
1	B	0.51	0/5007	0.59	0/6803
2	E	0.54	0/1446	0.64	0/1970
2	F	0.56	0/1446	0.63	1/1970 (0.1%)
All	All	0.52	0/12906	0.61	1/17546 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	330	ASN	N-CA-C	-5.03	97.41	111.00

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	4870	0	4643	208	0
1	B	4870	0	4643	209	1
2	E	1400	0	1329	46	1
2	F	1400	0	1329	45	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	12544	0	11944	507	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:CYS:HB2	1:A:488:VAL:CG2	1.87	1.03
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.42	1.01
1:B:261:CYS:HB2	1:B:488:VAL:HG13	1.42	1.00
1:B:74:LYS:HE2	1:B:106:SER:OG	1.64	0.95
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.47	0.94
1:A:233:ILE:HD11	1:A:581:VAL:HG21	1.52	0.89
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.54	0.88
1:A:261:CYS:HB2	1:A:488:VAL:HG23	1.56	0.85
2:F:372:THR:HG22	2:F:373:LYS:H	1.41	0.85
1:B:479:GLU:O	1:B:483:GLU:HB2	1.77	0.85
1:A:430:GLU:OE2	1:A:541:LYS:HD3	1.78	0.84
1:B:122:THR:O	1:B:126:ILE:HG23	1.79	0.83
1:A:55:THR:HG22	1:A:56:GLU:H	1.45	0.82
1:A:500:PRO:O	1:A:506:VAL:HG11	1.79	0.81
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.62	0.80
1:B:429:GLN:H	1:B:429:GLN:HE21	1.29	0.80
1:A:229:THR:HG23	1:A:516:TYR:OH	1.83	0.79
1:B:55:THR:HG22	1:B:56:GLU:H	1.48	0.78
1:A:31:LYS:HD3	1:A:35:GLU:OE2	1.82	0.78
1:A:285:PHE:HE1	1:A:436:ILE:HG21	1.48	0.78
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.48	0.78
1:A:514:ARG:HG2	1:A:515:TYR:N	1.99	0.77
2:E:372:THR:HG22	2:E:373:LYS:H	1.50	0.76
1:A:439:LEU:HB3	1:A:591:LEU:HD22	1.67	0.76
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.67	0.76
1:A:429:GLN:H	1:A:429:GLN:HE21	1.34	0.76
1:A:348:ALA:HB1	1:A:379:ILE:HD13	1.68	0.75
1:A:501:ALA:HA	1:A:506:VAL:HG11	1.69	0.74
1:B:553:LYS:HE3	1:B:573:VAL:O	1.87	0.74
1:A:476:LYS:O	1:A:480:MET:HG3	1.87	0.73
1:A:499:ASP:O	1:A:501:ALA:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:MET:CE	1:A:499:ASP:H	2.03	0.71
1:B:564:GLU:HB3	1:B:568:LEU:HD12	1.72	0.71
1:A:233:ILE:HD11	1:A:581:VAL:CG2	2.20	0.70
1:B:407:ILE:HD11	1:B:522:GLN:HA	1.74	0.70
1:B:549:GLU:H	1:B:549:GLU:CD	1.92	0.70
1:B:49:ASN:HB3	1:B:58:ASN:ND2	2.07	0.70
1:A:290:ASN:C	1:A:292:ASP:H	1.96	0.69
1:A:446:ILE:H	1:A:446:ILE:HD12	1.57	0.69
1:B:366:MET:HE1	1:B:441:LYS:HE3	1.74	0.69
1:A:338:ASN:HD22	1:A:338:ASN:H	1.40	0.69
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.28	0.68
1:B:103:ASN:HB3	1:B:107:VAL:HB	1.73	0.68
2:F:372:THR:HG22	2:F:373:LYS:N	2.06	0.68
1:B:290:ASN:C	1:B:292:ASP:H	1.95	0.68
1:A:474:MET:HE1	1:A:499:ASP:H	1.58	0.68
1:A:501:ALA:HA	1:A:506:VAL:CG1	2.23	0.68
2:E:388:VAL:CG2	2:E:495:ARG:HG2	2.24	0.68
1:B:178:PRO:O	1:B:181:GLU:HB2	1.94	0.68
1:B:47:SER:HA	1:B:62:MET:CG	2.23	0.68
1:B:440:LEU:HD13	1:B:444:LEU:HD22	1.74	0.67
1:B:252:TYR:CE2	1:B:266:LEU:HD22	2.29	0.67
1:B:49:ASN:HB3	1:B:58:ASN:HD22	1.59	0.67
2:F:406:ALA:HA	2:F:410:TYR:O	1.94	0.67
1:B:338:ASN:HD22	1:B:338:ASN:H	1.43	0.67
1:B:310:GLU:CG	1:B:421:ILE:HD11	2.24	0.67
1:A:459:TRP:O	1:A:463:VAL:HG23	1.95	0.67
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.60	0.66
1:A:493:HIS:HD2	1:A:499:ASP:OD2	1.78	0.66
1:B:338:ASN:HD22	1:B:338:ASN:N	1.93	0.66
1:B:365:THR:HG22	1:B:367:ASP:H	1.62	0.65
2:F:351:ASP:O	2:F:352:TYR:HB2	1.95	0.65
1:B:520:LEU:HD22	1:B:579:MET:HE3	1.78	0.65
1:A:521:TYR:HD1	1:A:521:TYR:H	1.45	0.65
1:B:526:GLN:NE2	1:B:526:GLN:HA	2.12	0.65
1:A:285:PHE:CE1	1:A:436:ILE:HG21	2.32	0.64
1:B:430:GLU:O	1:B:431:ASP:HB2	1.97	0.64
2:F:323:CYS:N	2:F:350:ALA:HB2	2.11	0.64
1:A:499:ASP:C	1:A:501:ALA:H	2.01	0.64
2:F:388:VAL:CG2	2:F:495:ARG:HG2	2.27	0.64
1:A:174:LYS:HG2	1:A:496:THR:O	1.98	0.64
1:A:489:GLU:HG2	1:A:613:TYR:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:SER:O	1:B:514:ARG:HD2	1.97	0.64
1:A:49:ASN:HB3	1:A:58:ASN:HD22	1.60	0.64
1:A:455:MET:HE1	1:A:481:LYS:HE2	1.80	0.64
1:B:265:HIS:ND1	1:B:490:PRO:HG3	2.14	0.63
1:B:520:LEU:HD22	1:B:579:MET:CE	2.28	0.63
1:B:177:ARG:HH22	1:B:495:GLU:HA	1.64	0.63
1:B:459:TRP:O	1:B:463:VAL:HG23	1.98	0.63
1:B:261:CYS:HB2	1:B:488:VAL:CG1	2.24	0.63
1:A:103:ASN:HB3	1:A:107:VAL:HB	1.80	0.63
1:A:72:PHE:O	1:A:76:GLN:HG2	1.99	0.62
1:B:72:PHE:O	1:B:76:GLN:HG2	1.99	0.62
1:A:505:HIS:HE1	1:A:515:TYR:OH	1.81	0.62
1:A:49:ASN:HB3	1:A:58:ASN:ND2	2.15	0.62
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.82	0.62
1:A:178:PRO:O	1:A:181:GLU:HB2	1.99	0.62
2:E:455:ILE:O	2:E:455:ILE:HG22	2.00	0.62
1:B:478:TRP:O	1:B:482:ARG:HG2	1.99	0.61
1:B:402:GLU:HB3	1:B:518:ARG:HG3	1.81	0.61
1:A:494:ASP:OD2	1:A:496:THR:HG22	2.01	0.61
1:A:597:ASP:O	1:A:600:LYS:HB2	2.00	0.61
2:F:355:LEU:H	2:F:355:LEU:HD12	1.65	0.61
1:A:111:ASP:O	1:A:114:LYS:HD3	2.01	0.61
1:A:338:ASN:HD22	1:A:338:ASN:N	1.99	0.61
2:E:388:VAL:HG22	2:E:495:ARG:HG2	1.82	0.61
1:A:400:PHE:HE2	1:A:557:MET:HE3	1.66	0.61
1:B:446:ILE:HG22	1:B:519:THR:HG23	1.82	0.61
1:B:310:GLU:HG2	1:B:421:ILE:HD11	1.81	0.61
1:A:177:ARG:NH1	1:A:470:LYS:O	2.33	0.61
2:F:388:VAL:HG22	2:F:495:ARG:HG2	1.84	0.60
2:F:327:GLU:O	2:F:331:ALA:HB2	2.01	0.60
1:B:174:LYS:HA	1:B:496:THR:O	2.00	0.60
1:A:400:PHE:CE2	1:A:557:MET:HE3	2.37	0.60
1:A:417:HIS:HB2	1:A:543:ASP:OD1	2.01	0.60
1:A:541:LYS:HB2	1:A:541:LYS:NZ	2.15	0.60
1:B:456:LEU:CD2	1:B:460:ARG:HD2	2.31	0.60
1:A:348:ALA:HB1	1:A:379:ILE:CD1	2.32	0.60
1:B:591:LEU:HG	1:B:595:LEU:HD22	1.84	0.60
2:E:472:PRO:O	2:E:473:ASN:HB2	2.02	0.59
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.37	0.59
2:E:327:GLU:O	2:E:331:ALA:HB2	2.01	0.59
2:E:455:ILE:HD12	2:E:455:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASN:OD1	1:B:582:ARG:HB2	2.02	0.59
1:A:310:GLU:CG	1:A:421:ILE:HD11	2.32	0.59
1:B:47:SER:HA	1:B:62:MET:HG3	1.85	0.59
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.84	0.59
1:B:20:THR:HG23	1:B:23:GLU:HB2	1.85	0.59
1:A:519:THR:O	1:A:522:GLN:HG2	2.03	0.59
2:E:337:VAL:HG22	2:E:388:VAL:O	2.03	0.58
1:A:457:GLU:OE1	1:A:460:ARG:NH1	2.36	0.58
1:B:117:ASN:O	1:B:121:ASN:HB2	2.03	0.58
1:B:366:MET:HE1	1:B:441:LYS:CE	2.33	0.58
1:A:209:VAL:HG21	1:A:565:PRO:HB3	1.85	0.58
1:A:555:PHE:HA	1:A:558:LEU:HB2	1.86	0.58
1:A:294:THR:O	1:A:298:VAL:HG23	2.03	0.58
1:A:545:SER:O	1:A:547:SER:N	2.37	0.57
1:A:39:LEU:O	1:A:39:LEU:HD23	2.05	0.57
1:B:526:GLN:HG3	1:B:539:LEU:HD11	1.85	0.57
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.86	0.57
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.85	0.57
1:B:378:HIS:CE1	1:B:402:GLU:OE1	2.56	0.57
1:A:514:ARG:HG2	1:A:515:TYR:H	1.69	0.57
1:B:47:SER:HA	1:B:62:MET:HG2	1.85	0.57
1:A:613:TYR:O	1:A:615:ASP:N	2.37	0.57
1:A:462:MET:HE2	1:A:468:ILE:HD11	1.86	0.57
2:E:337:VAL:CG2	2:E:389:VAL:HG12	2.35	0.57
1:B:289:PRO:O	1:B:290:ASN:C	2.43	0.57
1:B:431:ASP:C	1:B:433:GLU:H	2.08	0.57
1:B:31:LYS:HD3	1:B:35:GLU:OE2	2.04	0.57
2:E:341:GLU:O	2:E:385:ASP:HA	2.04	0.57
1:A:480:MET:O	1:A:484:ILE:HG12	2.05	0.57
2:F:372:THR:CG2	2:F:373:LYS:H	2.15	0.56
2:E:351:ASP:O	2:E:352:TYR:HB2	2.05	0.56
1:B:456:LEU:HD11	1:B:503:LEU:HD12	1.87	0.56
2:E:372:THR:HG22	2:E:373:LYS:N	2.18	0.56
1:B:21:ILE:HA	1:B:24:GLN:HG2	1.87	0.56
1:A:440:LEU:HD13	1:A:444:LEU:HD22	1.87	0.56
2:F:455:ILE:O	2:F:455:ILE:HG22	2.04	0.56
1:B:570:LEU:HD23	1:B:574:VAL:HG22	1.87	0.56
2:E:335:PRO:HG3	2:E:341:GLU:HG2	1.88	0.56
1:B:458:LYS:O	1:B:462:MET:HG3	2.05	0.56
1:B:56:GLU:HA	1:B:59:VAL:HG12	1.87	0.56
1:A:181:GLU:O	1:A:184:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:459:PRO:HB2	2:E:467:CYS:CB	2.36	0.56
1:A:541:LYS:HB2	1:A:541:LYS:HZ2	1.71	0.56
2:E:337:VAL:HG21	2:E:389:VAL:HG12	1.88	0.56
1:B:275:TRP:O	1:B:278:LEU:HB2	2.06	0.56
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.87	0.56
2:E:432:SER:HA	2:E:485:THR:HG22	1.89	0.55
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.70	0.55
1:B:440:LEU:HD13	1:B:444:LEU:CD2	2.36	0.55
1:B:407:ILE:HD11	1:B:522:GLN:O	2.06	0.55
1:A:393:ARG:O	1:A:394:ASN:HB2	2.07	0.55
1:A:56:GLU:HA	1:A:59:VAL:HG12	1.88	0.55
1:B:578:ASN:ND2	1:B:579:MET:H	2.05	0.55
2:F:356:TYR:OH	2:F:370:SER:O	2.24	0.55
1:B:524:GLN:HE22	1:B:579:MET:HA	1.70	0.55
1:A:122:THR:O	1:A:126:ILE:HG23	2.05	0.55
2:E:406:ALA:HA	2:E:410:TYR:O	2.07	0.55
1:B:418:LEU:O	1:B:421:ILE:HG22	2.06	0.54
1:A:169:ARG:HH12	1:A:271:TRP:HA	1.73	0.54
1:B:429:GLN:HE21	1:B:429:GLN:N	2.03	0.54
1:B:59:VAL:O	1:B:63:ASN:OD1	2.26	0.54
1:B:393:ARG:O	1:B:394:ASN:HB2	2.07	0.54
1:A:59:VAL:O	1:A:63:ASN:OD1	2.26	0.54
1:A:311:ALA:HA	1:A:373:HIS:CE1	2.42	0.54
1:A:538:PRO:HD2	1:A:541:LYS:NZ	2.23	0.54
1:A:352:GLY:O	1:A:353:LYS:HB2	2.07	0.54
1:B:251:ALA:O	1:B:253:PRO:HD3	2.06	0.54
1:A:55:THR:HG22	1:A:56:GLU:N	2.19	0.54
1:A:143:LEU:O	1:A:148:LEU:HB2	2.07	0.54
2:F:341:GLU:O	2:F:385:ASP:HA	2.07	0.54
1:B:448:GLY:O	1:B:451:PRO:HD2	2.07	0.54
1:A:213:ASP:HA	1:A:216:ASP:OD1	2.08	0.54
1:A:531:GLN:O	1:A:534:LYS:N	2.38	0.54
1:A:281:LEU:N	1:A:281:LEU:HD23	2.23	0.54
1:B:417:HIS:HB2	1:B:543:ASP:OD2	2.08	0.54
1:B:442:GLN:O	1:B:446:ILE:HG12	2.08	0.53
1:A:21:ILE:HA	1:A:24:GLN:HG2	1.89	0.53
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.44	0.53
1:A:462:MET:CE	1:A:468:ILE:HD11	2.38	0.53
1:B:294:THR:O	1:B:298:VAL:HG23	2.09	0.53
1:A:80:ALA:C	1:A:82:MET:H	2.10	0.53
2:F:329:PHE:CZ	2:F:355:LEU:HD23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:HA	1:A:114:LYS:HD2	1.90	0.53
1:B:143:LEU:O	1:B:148:LEU:HB2	2.08	0.53
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.91	0.53
1:A:397:ASN:HD21	1:A:521:TYR:HE2	1.57	0.53
1:A:168:TRP:NE1	1:A:502:SER:HB2	2.23	0.53
1:A:511:SER:O	1:A:514:ARG:HD2	2.09	0.52
2:E:425:THR:HG21	2:E:495:ARG:HG3	1.91	0.52
1:A:566:TRP:HZ3	1:A:570:LEU:HD12	1.74	0.52
1:B:556:ASN:O	1:B:559:ARG:HG2	2.09	0.52
1:A:233:ILE:CD1	1:A:581:VAL:HG21	2.33	0.52
1:B:366:MET:HE1	1:B:441:LYS:NZ	2.25	0.52
1:A:316:VAL:HA	1:A:320:LEU:O	2.10	0.51
1:A:261:CYS:CB	1:A:488:VAL:HG23	2.34	0.51
1:B:262:LEU:O	1:B:487:VAL:HG13	2.09	0.51
1:A:169:ARG:O	1:A:497:TYR:HD1	1.93	0.51
2:F:432:SER:HA	2:F:485:THR:HG22	1.92	0.51
1:B:261:CYS:CB	1:B:488:VAL:HG13	2.27	0.51
2:E:453:ARG:HG2	2:E:455:ILE:HD11	1.92	0.51
1:B:485:VAL:HG12	1:B:487:VAL:HG23	1.91	0.51
1:B:611:SER:HB2	1:B:614:ALA:HB3	1.92	0.51
2:F:326:GLY:O	2:F:330:ASN:HB2	2.10	0.51
2:E:323:CYS:N	2:E:350:ALA:HB2	2.25	0.51
2:F:346:SER:O	2:F:347:ASN:HB2	2.10	0.51
1:B:310:GLU:HG3	1:B:421:ILE:HD11	1.92	0.51
1:A:170:SER:O	1:A:174:LYS:HG3	2.10	0.51
2:E:483:PHE:CG	2:E:493:PRO:HG3	2.46	0.51
1:B:348:ALA:HB1	1:B:379:ILE:CD1	2.41	0.51
1:B:111:ASP:O	1:B:114:LYS:HD3	2.11	0.51
2:E:357:ASN:O	2:E:358:SER:HB2	2.10	0.51
1:B:290:ASN:C	1:B:292:ASP:N	2.60	0.51
1:A:310:GLU:HG2	1:A:421:ILE:HD11	1.91	0.51
2:F:483:PHE:CG	2:F:493:PRO:HG3	2.46	0.51
1:A:225:ASP:O	1:A:229:THR:HG22	2.11	0.51
1:B:338:ASN:ND2	1:B:338:ASN:H	2.07	0.51
2:F:455:ILE:N	2:F:455:ILE:HD12	2.26	0.51
1:B:406:GLU:HB3	1:B:522:GLN:OE1	2.11	0.51
1:A:429:GLN:N	1:A:429:GLN:HE21	2.04	0.51
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.51	0.50
1:A:482:ARG:HD3	1:A:608:THR:O	2.10	0.50
1:A:402:GLU:HB3	1:A:518:ARG:CD	2.28	0.50
2:F:334:PHE:CE2	2:F:386:SER:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:ARG:HB2	1:B:559:ARG:HH11	1.76	0.50
2:F:335:PRO:CG	2:F:341:GLU:HG2	2.35	0.50
1:B:20:THR:HG23	1:B:23:GLU:CB	2.41	0.50
2:F:390:LYS:HG2	2:F:490:GLY:O	2.12	0.50
1:A:472:GLN:O	1:A:476:LYS:HB2	2.11	0.50
1:B:263:PRO:HB2	1:B:266:LEU:HD12	1.93	0.50
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.94	0.50
2:F:324:PRO:HD3	2:F:348:CYS:SG	2.52	0.50
1:A:460:ARG:NE	1:A:506:VAL:HG22	2.26	0.50
1:A:555:PHE:O	1:A:559:ARG:HG2	2.12	0.50
1:B:134:ASN:HB3	1:B:137:ASN:HB3	1.94	0.50
1:B:476:LYS:O	1:B:480:MET:HG3	2.12	0.50
2:E:383:TYR:HB2	2:E:500:SER:HB2	1.94	0.50
1:B:414:THR:O	1:B:418:LEU:HD22	2.12	0.49
1:A:394:ASN:HD22	1:A:395:GLY:H	1.58	0.49
1:B:50:TYR:HE1	1:B:54:ILE:HG23	1.76	0.49
1:A:166:GLU:OE1	1:A:493:HIS:CE1	2.65	0.49
1:A:290:ASN:C	1:A:292:ASP:N	2.60	0.49
1:B:184:VAL:O	1:B:188:ASN:HB2	2.12	0.49
1:B:611:SER:CB	1:B:614:ALA:HB3	2.43	0.49
1:A:499:ASP:C	1:A:501:ALA:N	2.63	0.49
1:A:257:SER:HB2	1:A:610:TRP:CE2	2.48	0.49
2:F:471:ALA:O	2:F:474:CYS:HB2	2.13	0.49
2:F:453:ARG:NH1	2:F:455:ILE:HD11	2.28	0.49
1:A:165:TRP:HZ2	1:A:478:TRP:HH2	1.60	0.49
1:B:468:ILE:HG22	1:B:473:TRP:HD1	1.77	0.49
1:B:39:LEU:HD22	1:B:69:TRP:HE3	1.77	0.49
1:B:159:ASN:HA	1:B:162:LEU:HB3	1.94	0.49
1:B:51:ASN:ND2	1:B:343:VAL:HG11	2.28	0.49
1:B:499:ASP:O	1:B:502:SER:HB2	2.12	0.49
1:B:51:ASN:HD22	1:B:343:VAL:HG11	1.78	0.49
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.48	0.48
1:A:30:ASP:O	1:A:34:HIS:HD2	1.96	0.48
1:B:538:PRO:HB2	1:B:540:HIS:CE1	2.48	0.48
1:A:240:LEU:CD2	1:A:244:VAL:HG23	2.43	0.48
1:B:168:TRP:O	1:B:172:VAL:HG22	2.13	0.48
1:B:518:ARG:O	1:B:522:GLN:HB2	2.13	0.48
1:A:47:SER:HA	1:A:62:MET:CG	2.43	0.48
1:B:348:ALA:HB1	1:B:379:ILE:HD13	1.95	0.48
1:B:88:ILE:HG21	1:B:93:VAL:HG23	1.96	0.48
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ASP:N	1:A:500:PRO:HD2	2.28	0.48
1:A:135:PRO:HD3	1:A:163:TRP:CZ2	2.49	0.48
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.95	0.48
2:F:338:TYR:HE1	2:F:455:ILE:HG23	1.78	0.48
1:A:252:TYR:CE2	1:A:266:LEU:HD22	2.49	0.48
1:B:407:ILE:HG23	1:B:526:GLN:NE2	2.29	0.47
1:B:177:ARG:O	1:B:181:GLU:HG2	2.14	0.47
1:A:414:THR:HG21	1:A:541:LYS:O	2.14	0.47
2:E:396:GLN:OE1	2:E:403:GLY:O	2.33	0.47
1:B:394:ASN:HD22	1:B:395:GLY:H	1.62	0.47
2:E:489:ILE:HD13	2:E:492:GLN:NE2	2.29	0.47
1:B:248:LEU:HD12	1:B:262:LEU:HD22	1.97	0.47
1:B:600:LYS:HE3	1:B:601:ASN:HD21	1.80	0.47
1:B:169:ARG:O	1:B:173:GLY:HA3	2.15	0.47
1:B:464:PHE:C	1:B:466:GLY:H	2.18	0.47
1:A:24:GLN:HG3	1:A:83:TYR:HE2	1.80	0.47
1:A:280:SER:HB2	1:A:281:LEU:HD23	1.95	0.47
1:A:463:VAL:HG12	1:A:463:VAL:O	2.14	0.47
1:B:594:TRP:CE3	1:B:595:LEU:HD13	2.49	0.47
1:B:30:ASP:O	1:B:34:HIS:HD2	1.98	0.47
1:A:471:ASP:HA	1:A:495:GLU:HG3	1.96	0.47
1:A:351:LEU:HD22	1:A:355:ASP:OD1	2.15	0.46
1:A:402:GLU:CB	1:A:518:ARG:HD2	2.30	0.46
2:F:425:THR:HG21	2:F:495:ARG:HG3	1.97	0.46
2:E:483:PHE:HB3	2:E:493:PRO:HG3	1.97	0.46
1:B:144:LEU:HB2	1:B:168:TRP:CH2	2.50	0.46
1:A:430:GLU:O	1:A:431:ASP:CB	2.63	0.46
1:B:505:HIS:H	1:B:505:HIS:CD2	2.32	0.46
1:A:30:ASP:O	1:A:34:HIS:CD2	2.69	0.46
2:F:351:ASP:O	2:F:352:TYR:CB	2.63	0.46
1:A:396:ALA:HB3	1:A:400:PHE:CD1	2.51	0.46
1:B:24:GLN:HG3	1:B:83:TYR:HE2	1.81	0.46
1:A:271:TRP:CD2	1:A:503:LEU:HD23	2.51	0.46
1:A:168:TRP:HE1	1:A:502:SER:HB2	1.81	0.46
1:A:201:ASP:O	1:A:219:ARG:HD2	2.16	0.46
2:E:437:ASN:O	2:E:439:LYS:HG3	2.15	0.46
1:A:446:ILE:N	1:A:446:ILE:HD12	2.29	0.46
1:B:366:MET:CE	1:B:441:LYS:NZ	2.78	0.46
1:B:366:MET:CE	1:B:441:LYS:HE3	2.45	0.46
1:A:545:SER:C	1:A:547:SER:H	2.19	0.46
1:A:433:GLU:O	1:A:436:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HB3	1:A:93:VAL:CG2	2.45	0.46
1:B:344:CYS:O	1:B:345:HIS:C	2.54	0.46
1:A:194:ASN:O	1:A:195:HIS:HB2	2.15	0.46
1:B:251:ALA:C	1:B:253:PRO:HD3	2.37	0.46
1:B:460:ARG:NE	1:B:506:VAL:HG22	2.31	0.45
1:A:338:ASN:H	1:A:338:ASN:ND2	2.12	0.45
1:B:176:LEU:HD13	1:B:501:ALA:HB1	1.98	0.45
1:B:600:LYS:HE3	1:B:601:ASN:ND2	2.32	0.45
2:F:403:GLY:HA2	2:F:407:ASP:CG	2.37	0.45
1:B:311:ALA:HA	1:B:373:HIS:CE1	2.52	0.45
1:A:251:ALA:O	1:A:253:PRO:HD3	2.16	0.45
2:F:387:PHE:CE1	2:F:496:VAL:HB	2.51	0.45
2:F:373:LYS:NZ	2:F:375:ASN:HD22	2.14	0.45
1:B:204:ARG:NE	1:B:223:ILE:HD11	2.31	0.45
1:B:289:PRO:O	1:B:290:ASN:O	2.34	0.45
1:A:507:SER:C	1:A:508:ASN:HD22	2.20	0.45
1:A:581:VAL:HG23	1:A:584:LEU:HD23	1.97	0.45
1:B:557:MET:HB3	1:B:573:VAL:HG22	1.98	0.45
1:A:327:PHE:CE2	1:A:358:ILE:HG13	2.45	0.45
1:A:517:THR:HB	1:A:521:TYR:CE1	2.51	0.45
1:A:394:ASN:HD22	1:A:395:GLY:N	2.14	0.45
1:B:611:SER:H	1:B:615:ASP:HB3	1.81	0.45
1:A:581:VAL:CG2	1:A:584:LEU:HD23	2.46	0.45
1:A:516:TYR:CD2	1:A:516:TYR:C	2.90	0.45
1:B:521:TYR:O	1:B:522:GLN:C	2.56	0.45
1:B:181:GLU:O	1:B:184:VAL:HG22	2.16	0.45
1:A:24:GLN:NE2	2:E:473:ASN:HD21	2.14	0.45
1:B:291:ILE:HG22	1:B:291:ILE:O	2.17	0.45
1:B:557:MET:HG2	1:B:573:VAL:HG21	1.99	0.45
1:B:306:ARG:O	1:B:310:GLU:HB2	2.17	0.44
2:F:483:PHE:HB3	2:F:493:PRO:HG3	2.00	0.44
2:E:367:TYR:HB2	2:E:417:MET:HB3	1.99	0.44
1:A:333:LEU:O	1:A:362:THR:HB	2.17	0.44
2:E:352:TYR:O	2:E:355:LEU:HD12	2.16	0.44
1:B:111:ASP:HA	1:B:114:LYS:HD2	1.99	0.44
1:B:240:LEU:CD2	1:B:244:VAL:HG23	2.47	0.44
1:A:589:GLU:N	1:A:590:PRO:CD	2.80	0.44
1:B:480:MET:HA	1:B:483:GLU:HB2	1.99	0.44
1:B:351:LEU:HD22	1:B:355:ASP:OD1	2.18	0.44
1:B:429:GLN:H	1:B:429:GLN:NE2	2.07	0.44
1:A:557:MET:HE2	1:A:557:MET:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PHE:CD2	1:A:557:MET:HE1	2.52	0.44
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.81	0.44
2:E:469:PRO:HA	2:E:471:ALA:H	1.82	0.44
1:B:501:ALA:HA	1:B:506:VAL:HG12	2.00	0.44
1:A:169:ARG:O	1:A:173:GLY:HA3	2.17	0.44
1:B:30:ASP:O	1:B:34:HIS:CD2	2.71	0.44
1:B:126:ILE:HD11	1:B:176:LEU:HG	2.00	0.44
1:B:134:ASN:CB	1:B:137:ASN:HB3	2.48	0.44
1:A:44:SER:HB3	1:A:351:LEU:HG	1.99	0.44
1:B:535:HIS:CD2	1:B:542:CYS:HB2	2.53	0.44
1:A:99:ALA:O	1:A:102:GLN:HG2	2.18	0.43
2:F:453:ARG:HG2	2:F:455:ILE:HD11	2.00	0.43
1:B:374:HIS:HA	1:B:405:GLY:O	2.18	0.43
1:B:290:ASN:O	1:B:292:ASP:N	2.52	0.43
1:B:430:GLU:O	1:B:431:ASP:CB	2.66	0.43
1:A:145:GLU:HA	1:A:146:PRO:HA	1.84	0.43
1:B:39:LEU:O	1:B:39:LEU:HD23	2.17	0.43
2:F:435:ASN:ND2	2:F:437:ASN:H	2.15	0.43
1:B:63:ASN:O	1:B:67:ASP:N	2.52	0.43
1:A:439:LEU:HD21	1:A:540:HIS:CD2	2.54	0.43
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.85	0.43
1:A:257:SER:HA	1:A:258:PRO:HD3	1.90	0.43
1:A:184:VAL:O	1:A:188:ASN:HB2	2.18	0.43
1:A:461:TRP:O	1:A:464:PHE:HB2	2.19	0.43
1:A:462:MET:C	1:A:464:PHE:H	2.20	0.43
1:A:468:ILE:HA	1:A:469:PRO:HD3	1.84	0.43
1:A:146:PRO:O	1:A:148:LEU:N	2.52	0.43
1:B:281:LEU:HD23	1:B:281:LEU:N	2.34	0.43
1:B:226:VAL:O	1:B:229:THR:HG22	2.19	0.43
1:A:482:ARG:NE	1:A:488:VAL:HG13	2.34	0.43
1:A:581:VAL:O	1:A:581:VAL:HG22	2.19	0.43
1:A:591:LEU:HG	1:A:595:LEU:HD21	1.99	0.43
1:A:83:TYR:HA	1:A:84:PRO:HD3	1.84	0.43
1:A:504:PHE:C	1:A:504:PHE:CD2	2.91	0.43
1:A:47:SER:HA	1:A:62:MET:HG2	2.01	0.43
1:B:41:TYR:CG	1:B:353:LYS:HG3	2.54	0.43
2:F:489:ILE:HD13	2:F:492:GLN:NE2	2.34	0.43
1:B:80:ALA:C	1:B:82:MET:H	2.22	0.43
1:B:316:VAL:HA	1:B:320:LEU:O	2.19	0.43
1:B:55:THR:HG22	1:B:56:GLU:N	2.26	0.43
1:B:155:SER:O	1:B:161:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:VAL:HB	1:B:492:PRO:HD2	2.01	0.43
1:A:249:MET:HG2	1:A:256:ILE:HB	1.99	0.43
1:B:385:TYR:CD2	1:B:385:TYR:C	2.92	0.43
1:B:408:MET:C	1:B:410:LEU:N	2.71	0.43
1:B:175:GLN:O	1:B:178:PRO:HD2	2.19	0.42
2:F:337:VAL:CG2	2:F:389:VAL:HG12	2.49	0.42
1:A:380:GLN:HA	1:A:383:MET:HE2	2.01	0.42
1:A:323:MET:HE3	1:A:376:MET:SD	2.59	0.42
1:B:381:TYR:CD2	1:B:558:LEU:HG	2.54	0.42
1:B:104:GLY:O	1:B:107:VAL:HG12	2.20	0.42
2:F:397:ILE:N	2:F:397:ILE:HD12	2.34	0.42
1:A:415:PRO:O	1:A:419:LYS:HB2	2.20	0.42
1:A:446:ILE:HG21	1:A:523:PHE:HE2	1.85	0.42
2:E:390:LYS:HG2	2:E:490:GLY:O	2.19	0.42
1:A:275:TRP:O	1:A:278:LEU:HB2	2.19	0.42
2:F:422:ALA:HA	2:F:495:ARG:O	2.19	0.42
1:B:446:ILE:HG22	1:B:519:THR:CG2	2.49	0.42
1:A:524:GLN:HE22	1:A:579:MET:HA	1.84	0.42
1:B:478:TRP:C	1:B:480:MET:N	2.70	0.42
1:B:403:ALA:O	1:B:407:ILE:HG12	2.20	0.42
1:B:209:VAL:HG13	1:B:217:TYR:N	2.35	0.42
1:A:21:ILE:HD13	1:A:21:ILE:N	2.35	0.42
1:B:580:ASN:OD1	1:B:583:PRO:HD3	2.20	0.42
1:B:169:ARG:HH12	1:B:271:TRP:HA	1.84	0.42
2:E:435:ASN:ND2	2:E:437:ASN:H	2.17	0.42
1:B:99:ALA:O	1:B:102:GLN:HG2	2.20	0.42
1:A:521:TYR:CD1	1:A:521:TYR:N	2.84	0.42
1:A:553:LYS:O	1:A:556:ASN:HB2	2.20	0.42
2:E:405:ILE:HA	2:E:409:ASN:HD22	1.84	0.42
1:A:326:GLY:HA2	1:A:329:GLU:HB3	2.01	0.42
1:A:55:THR:CG2	1:A:56:GLU:H	2.25	0.42
1:B:526:GLN:HE21	1:B:526:GLN:CA	2.18	0.42
1:A:545:SER:C	1:A:547:SER:N	2.73	0.42
1:B:600:LYS:HB2	1:B:600:LYS:NZ	2.34	0.42
1:B:388:GLN:HB3	1:B:389:PRO:HD2	2.02	0.42
1:B:570:LEU:HD23	1:B:574:VAL:CG2	2.49	0.42
1:B:379:ILE:O	1:B:383:MET:HG3	2.20	0.42
1:B:203:TRP:C	1:B:205:GLY:N	2.73	0.42
1:B:489:GLU:HA	1:B:490:PRO:HD3	1.90	0.41
2:E:416:PHE:O	2:E:417:MET:CB	2.69	0.41
1:A:365:THR:HG22	1:A:367:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TRP:NE1	1:A:306:ARG:NH1	2.68	0.41
1:B:407:ILE:HD11	1:B:522:GLN:CA	2.47	0.41
1:A:521:TYR:N	1:A:521:TYR:HD1	2.14	0.41
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.49	0.41
2:E:415:ASP:HB3	2:E:416:PHE:CD1	2.55	0.41
1:A:523:PHE:CD2	1:A:584:LEU:HD13	2.54	0.41
1:A:271:TRP:CE2	1:A:503:LEU:HD23	2.55	0.41
1:B:369:PHE:CD1	1:B:370:LEU:HD23	2.55	0.41
2:E:346:SER:O	2:E:347:ASN:HB2	2.21	0.41
2:E:353:SER:HA	2:E:356:TYR:HB2	2.03	0.41
1:A:111:ASP:HA	1:A:114:LYS:CD	2.49	0.41
1:B:21:ILE:HD13	1:B:22:GLU:H	1.86	0.41
1:B:395:GLY:O	1:B:396:ALA:C	2.59	0.41
1:B:611:SER:HA	1:B:612:PRO:HD3	1.96	0.41
1:B:116:LEU:HD13	1:B:186:LEU:HB2	2.03	0.41
1:A:611:SER:HA	1:A:612:PRO:HD3	1.87	0.41
1:B:126:ILE:C	1:B:126:ILE:HD12	2.40	0.41
1:B:177:ARG:HG2	1:B:495:GLU:O	2.21	0.41
1:A:520:LEU:O	1:A:521:TYR:C	2.58	0.41
1:B:265:HIS:ND1	1:B:490:PRO:CG	2.81	0.41
1:B:144:LEU:HD22	1:B:168:TRP:CZ2	2.56	0.41
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.91	0.41
1:A:400:PHE:CE2	1:A:557:MET:CE	3.02	0.41
1:B:170:SER:O	1:B:174:LYS:HG3	2.21	0.41
2:F:390:LYS:HB2	2:F:481:TYR:CE2	2.56	0.41
1:B:474:MET:SD	1:B:500:PRO:HD2	2.61	0.41
1:B:134:ASN:HB3	1:B:137:ASN:H	1.85	0.41
1:A:351:LEU:HD12	1:A:351:LEU:N	2.36	0.41
1:B:214:GLY:O	1:B:577:LYS:HD3	2.20	0.41
2:F:367:TYR:CD1	2:F:367:TYR:N	2.88	0.41
1:A:489:GLU:HA	1:A:490:PRO:HD3	1.92	0.41
1:A:613:TYR:CD1	1:A:614:ALA:N	2.89	0.41
1:B:514:ARG:HG2	1:B:515:TYR:N	2.36	0.41
1:A:56:GLU:O	1:A:60:GLN:HB2	2.20	0.41
1:A:591:LEU:HG	1:A:595:LEU:CD2	2.51	0.41
1:A:490:PRO:O	1:A:613:TYR:HB3	2.21	0.41
1:A:503:LEU:O	1:A:504:PHE:C	2.59	0.41
1:B:559:ARG:NH1	1:B:559:ARG:HB2	2.36	0.41
2:F:417:MET:CE	2:F:417:MET:HA	2.51	0.41
2:F:372:THR:CG2	2:F:373:LYS:N	2.76	0.41
1:A:379:ILE:O	1:A:383:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:THR:OG1	1:B:581:VAL:HB	2.21	0.41
1:B:385:TYR:C	1:B:385:TYR:HD2	2.24	0.41
2:E:390:LYS:HB2	2:E:481:TYR:CE2	2.56	0.41
1:B:440:LEU:HD13	1:B:440:LEU:C	2.41	0.40
1:A:126:ILE:HD11	1:A:176:LEU:HG	2.03	0.40
1:B:499:ASP:N	1:B:500:PRO:HD2	2.36	0.40
2:E:397:ILE:N	2:E:397:ILE:HD12	2.36	0.40
1:A:403:ALA:O	1:A:407:ILE:HG12	2.20	0.40
2:E:372:THR:CG2	2:E:373:LYS:H	2.27	0.40
2:E:403:GLY:HA2	2:E:407:ASP:CG	2.42	0.40
1:A:251:ALA:C	1:A:253:PRO:HD3	2.42	0.40
1:A:430:GLU:O	1:A:431:ASP:HB3	2.21	0.40
1:B:446:ILE:O	1:B:449:THR:HG22	2.21	0.40
2:F:489:ILE:HD13	2:F:492:GLN:HE22	1.86	0.40
1:B:74:LYS:HZ2	1:B:78:THR:HG21	1.86	0.40
1:A:460:ARG:HH21	1:A:506:VAL:HA	1.87	0.40
1:B:418:LEU:C	1:B:421:ILE:HG22	2.42	0.40
1:A:265:HIS:ND1	1:A:490:PRO:HG3	2.36	0.40
1:B:489:GLU:N	1:B:489:GLU:OE2	2.47	0.40
1:A:538:PRO:HD2	1:A:541:LYS:HZ3	1.85	0.40
2:E:435:ASN:ND2	2:E:435:ASN:C	2.75	0.40
2:F:337:VAL:HG21	2:F:389:VAL:HG12	2.03	0.40
2:E:326:GLY:O	2:E:330:ASN:HB2	2.21	0.40
1:A:580:ASN:ND2	1:A:583:PRO:HD3	2.36	0.40
1:B:296:ALA:O	1:B:300:GLN:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLN:NE2	2:E:469:PRO:O[2_556]	2.16	0.04

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%)	504 (85%)	71 (12%)	20 (3%)	5 25
1	B	595/603 (99%)	498 (84%)	78 (13%)	19 (3%)	5 27
2	E	170/186 (91%)	131 (77%)	25 (15%)	14 (8%)	1 5
2	F	170/186 (91%)	130 (76%)	27 (16%)	13 (8%)	1 6
All	All	1530/1578 (97%)	1263 (82%)	201 (13%)	66 (4%)	3 19

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	PRO
1	A	430	GLU
1	A	546	ASN
1	A	614	ALA
1	B	396	ALA
1	B	430	GLU
2	E	330	ASN
2	E	348	CYS
2	E	370	SER
2	E	373	LYS
2	E	402	THR
2	E	416	PHE
2	F	330	ASN
2	F	348	CYS
2	F	370	SER
2	F	373	LYS
2	F	402	THR
1	A	104	GLY
1	A	264	ALA
1	A	390	PHE
1	A	396	ALA
1	B	290	ASN
1	B	390	PHE
1	B	509	ASP
1	B	537	GLY
1	B	613	TYR
2	E	358	SER
2	E	401	GLN
2	E	415	ASP
2	F	347	ASN

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Mol	Chain	Res	Type
2	F	369	VAL
2	F	401	GLN
2	F	416	PHE
1	A	81	GLN
1	A	146	PRO
1	A	147	GLY
1	A	171	GLU
1	A	394	ASN
1	A	431	ASP
1	A	498	CYS
1	B	147	GLY
1	B	291	ILE
1	B	394	ASN
1	B	522	GLN
2	E	481	TYR
1	B	81	GLN
1	B	146	PRO
1	B	171	GLU
1	B	431	ASP
1	B	470	LYS
1	B	473	TRP
2	E	347	ASN
2	E	369	VAL
2	F	415	ASP
2	F	481	TYR
1	A	195	HIS
1	A	291	ILE
2	F	463	ASP
1	A	339	VAL
1	B	289	PRO
2	E	328	VAL
2	E	404	VAL
1	B	119	ILE
2	F	328	VAL
1	A	54	ILE
1	A	537	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	527/533 (99%)	487 (92%)	40 (8%)	16 51
1	B	527/533 (99%)	484 (92%)	43 (8%)	14 46
2	E	151/163 (93%)	140 (93%)	11 (7%)	17 52
2	F	151/163 (93%)	140 (93%)	11 (7%)	17 52
All	All	1356/1392 (97%)	1251 (92%)	105 (8%)	16 50

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ILE
1	A	62	MET
1	A	63	ASN
1	A	85	LEU
1	A	114	LYS
1	A	149	ASN
1	A	150	GLU
1	A	240	LEU
1	A	273	ARG
1	A	280	SER
1	A	281	LEU
1	A	317	SER
1	A	333	LEU
1	A	338	ASN
1	A	341	LYS
1	A	379	ILE
1	A	381	TYR
1	A	385	TYR
1	A	394	ASN
1	A	401	HIS
1	A	418	LEU
1	A	419	LYS
1	A	429	GLN
1	A	439	LEU
1	A	444	LEU
1	A	460	ARG
1	A	473	TRP
1	A	484	ILE
1	A	503	LEU

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Mol	Chain	Res	Type
1	A	514	ARG
1	A	521	TYR
1	A	526	GLN
1	A	549	GLU
1	A	557	MET
1	A	558	LEU
1	A	559	ARG
1	A	568	LEU
1	A	585	LEU
1	A	608	THR
1	B	20	THR
1	B	21	ILE
1	B	31	LYS
1	B	53	ASN
1	B	62	MET
1	B	89	GLN
1	B	114	LYS
1	B	118	THR
1	B	221	GLN
1	B	240	LEU
1	B	273	ARG
1	B	280	SER
1	B	281	LEU
1	B	317	SER
1	B	338	ASN
1	B	341	LYS
1	B	381	TYR
1	B	385	TYR
1	B	394	ASN
1	B	401	HIS
1	B	418	LEU
1	B	429	GLN
1	B	431	ASP
1	B	435	GLU
1	B	436	ILE
1	B	444	LEU
1	B	446	ILE
1	B	455	MET
1	B	473	TRP
1	B	483	GLU
1	B	484	ILE
1	B	493	HIS

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Mol	Chain	Res	Type
1	B	495	GLU
1	B	503	LEU
1	B	518	ARG
1	B	526	GLN
1	B	557	MET
1	B	559	ARG
1	B	573	VAL
1	B	578	ASN
1	B	585	LEU
1	B	595	LEU
1	B	600	LYS
2	E	323	CYS
2	E	329	PHE
2	E	355	LEU
2	E	356	TYR
2	E	364	PHE
2	E	412	LEU
2	E	417	MET
2	E	423	TRP
2	E	427	ASN
2	E	467	CYS
2	E	475	TYR
2	F	323	CYS
2	F	329	PHE
2	F	334	PHE
2	F	355	LEU
2	F	356	TYR
2	F	364	PHE
2	F	412	LEU
2	F	417	MET
2	F	423	TRP
2	F	427	ASN
2	F	475	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	42	GLN
1	A	49	ASN
1	A	53	ASN

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Mol	Chain	Res	Type
1	A	58	ASN
1	A	63	ASN
1	A	101	GLN
1	A	154	ASN
1	A	277	ASN
1	A	300	GLN
1	A	338	ASN
1	A	373	HIS
1	A	394	ASN
1	A	429	GLN
1	A	472	GLN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	524	GLN
1	A	526	GLN
1	A	535	HIS
1	A	540	HIS
1	A	586	ASN
1	A	599	ASN
1	B	24	GLN
1	B	33	ASN
1	B	42	GLN
1	B	49	ASN
1	B	51	ASN
1	B	53	ASN
1	B	58	ASN
1	B	63	ASN
1	B	101	GLN
1	B	154	ASN
1	B	195	HIS
1	B	277	ASN
1	B	300	GLN
1	B	338	ASN
1	B	373	HIS
1	B	394	ASN
1	B	429	GLN
1	B	505	HIS
1	B	524	GLN
1	B	526	GLN
1	B	531	GLN
1	B	535	HIS

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Mol	Chain	Res	Type
1	B	556	ASN
1	B	572	ASN
1	B	578	ASN
1	B	586	ASN
1	B	599	ASN
1	B	601	ASN
2	E	375	ASN
2	E	435	ASN
2	F	375	ASN
2	F	435	ASN
2	F	445	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 carbohydrates 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

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	597/603 (99%)	-0.16	6 (1%) 84 60	42, 76, 124, 151	0
1	B	597/603 (99%)	-0.04	11 (1%) 71 43	47, 81, 127, 151	0
2	E	174/186 (93%)	0.16	8 (4%) 36 14	64, 89, 135, 144	0
2	F	174/186 (93%)	0.08	6 (3%) 49 21	67, 90, 134, 145	0
All	All	1542/1578 (97%)	-0.05	31 (2%) 68 39	42, 82, 132, 151	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	ASP	5.4
2	E	501	PHE	4.2
2	E	500	SER	3.6
1	B	615	ASP	3.4
2	E	357	ASN	3.4
1	A	84	PRO	3.3
1	B	135	PRO	3.3
1	A	138	PRO	3.1
1	B	338	ASN	3.1
2	F	364	PHE	2.7
1	A	298	VAL	2.7
1	B	64	ASN	2.6
1	B	614	ALA	2.6
2	F	360	PHE	2.6
2	F	443	LEU	2.5
2	E	355	LEU	2.5
1	B	139	GLN	2.5
2	E	382	VAL	2.4
1	A	108	LEU	2.4
2	F	477	PRO	2.3
2	F	350	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	339	VAL	2.3
2	F	354	VAL	2.3
2	E	364	PHE	2.2
1	B	140	GLU	2.2
2	E	359	THR	2.2
1	A	75	GLU	2.1
1	B	137	ASN	2.1
1	B	134	ASN	2.0
1	A	290	ASN	2.0
2	E	345	ILE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	A	902	1/1	0.89	0.50	11.62	96,96,96,96	0
4	CL	B	902	1/1	0.82	0.22	-0.11	114,114,114,114	0
3	ZN	B	901	1/1	0.83	0.39	-	83,83,83,83	0
3	ZN	A	901	1/1	0.94	0.34	-	82,82,82,82	0

6.5 Other polymers

There are no such residues in this entry.