Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2023 – 01:47 PM EDT

PDB ID	:	8GB2
Title	:	Crystal structure of Apo-SAMHD1
Authors	:	Egleston, M.; Dong, L.; Howlader, A.H.; Bhat, S.; Orris, B.; Bianchet, M.A.; Greenberg, M.M.; Stivers, J.T.
Deposited on	:	2023-02-24
Resolution	:	3.07 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:

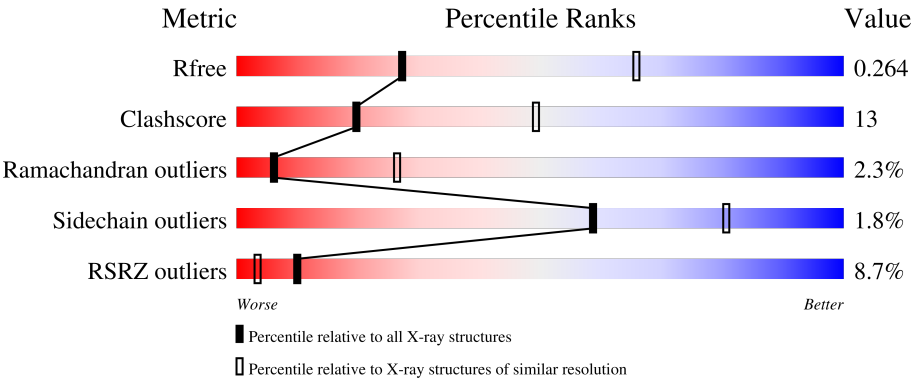
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	516	65% 20% · 14%
1	B	516	11% 59% 25% · 14%
1	C	516	18% 49% 34% · 13%
1	D	516	% 67% 17% · 14%

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
2	FE	D	701	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28956 atoms, of which 14422 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	445	Total	C	H	N	O	S	0	0	0
			7243	2326	3607	633	658	19			
1	A	443	Total	C	H	N	O	S	0	0	0
			7224	2323	3601	631	650	19			
1	B	442	Total	C	H	N	O	S	0	0	0
			7203	2314	3589	630	651	19			
1	C	447	Total	C	H	N	O	S	0	0	0
			7281	2340	3625	636	660	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	111	SER	-	expression tag	UNP Q9Y3Z3
D	112	MET	-	expression tag	UNP Q9Y3Z3
A	111	SER	-	expression tag	UNP Q9Y3Z3
A	112	MET	-	expression tag	UNP Q9Y3Z3
B	111	SER	-	expression tag	UNP Q9Y3Z3
B	112	MET	-	expression tag	UNP Q9Y3Z3
C	111	SER	-	expression tag	UNP Q9Y3Z3
C	112	MET	-	expression tag	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

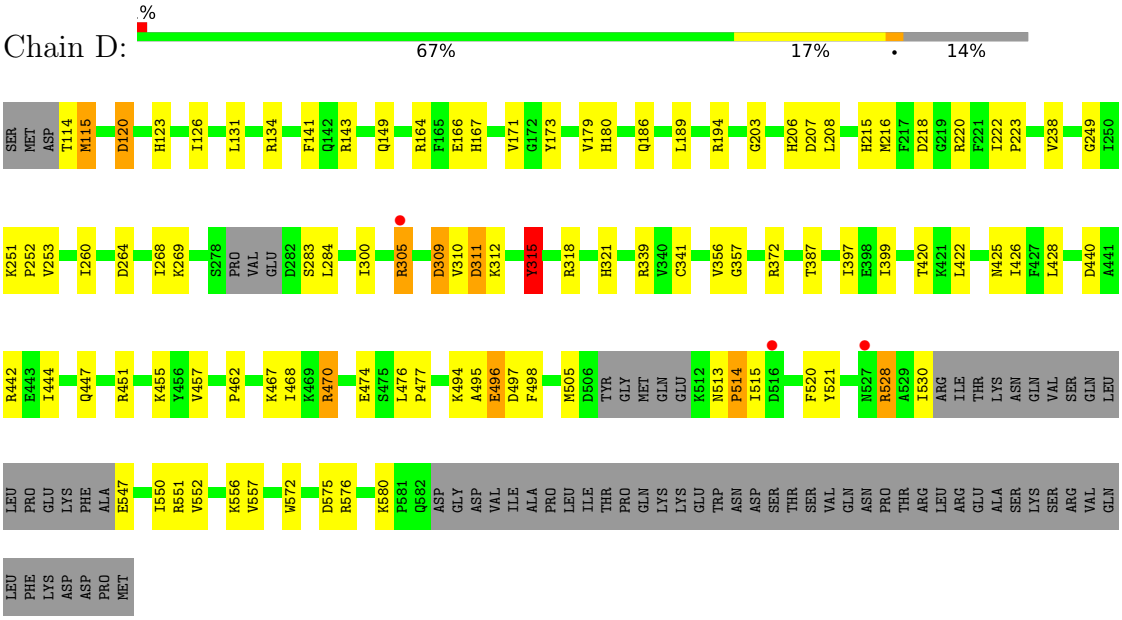
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

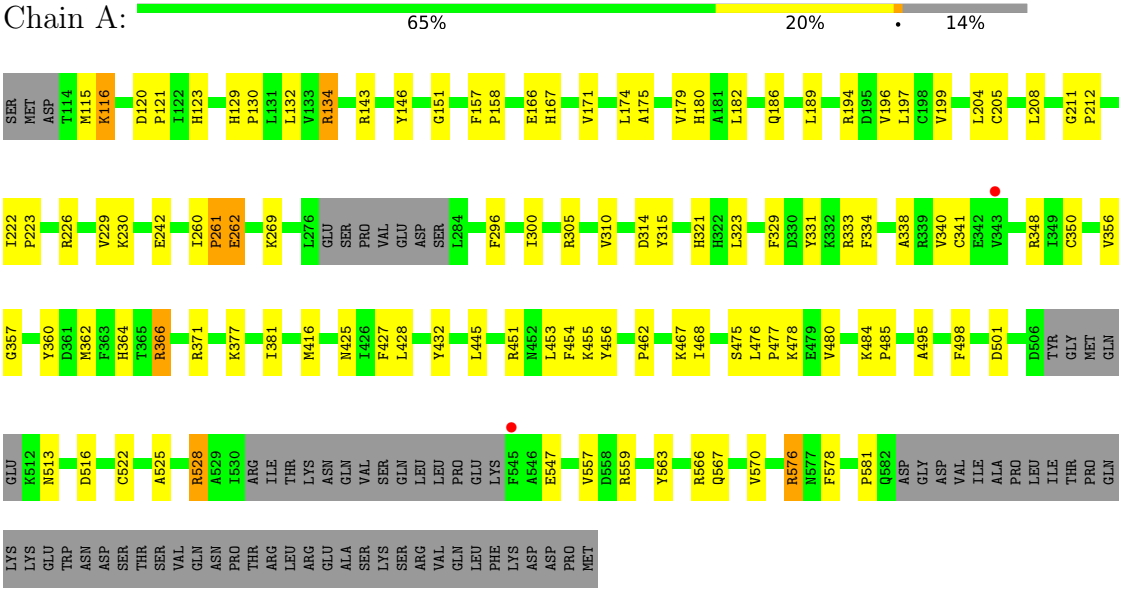
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



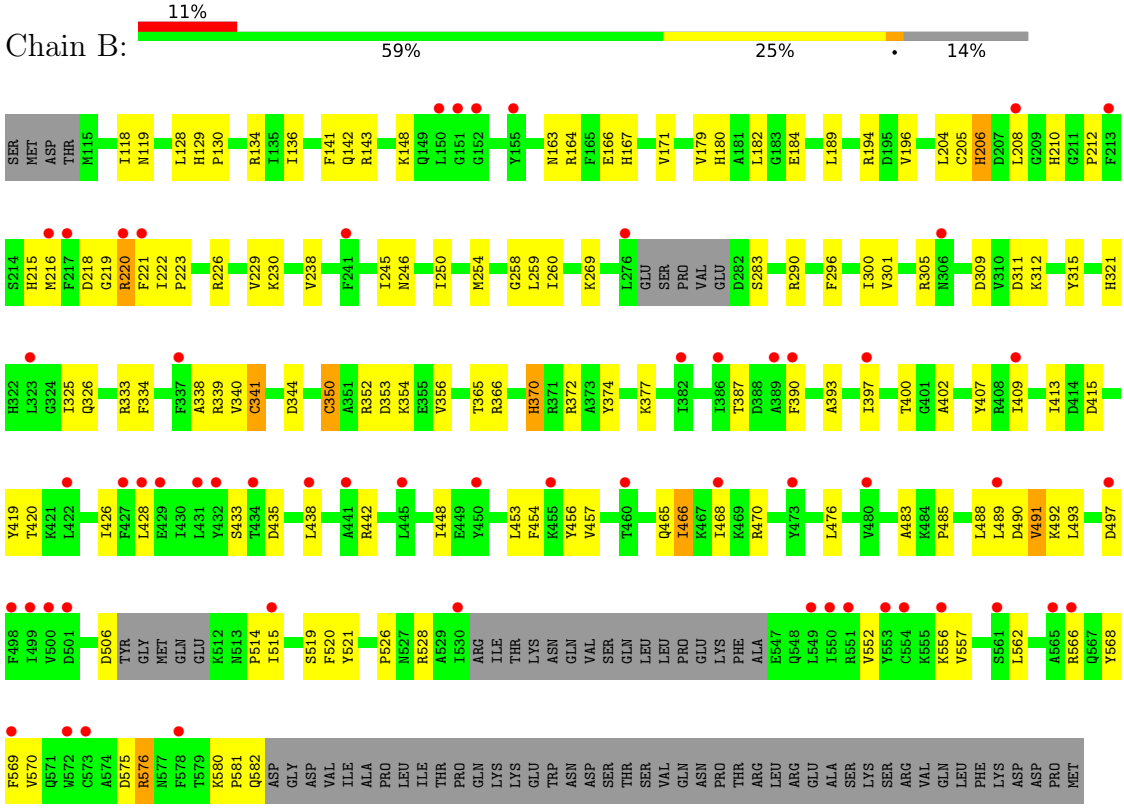
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



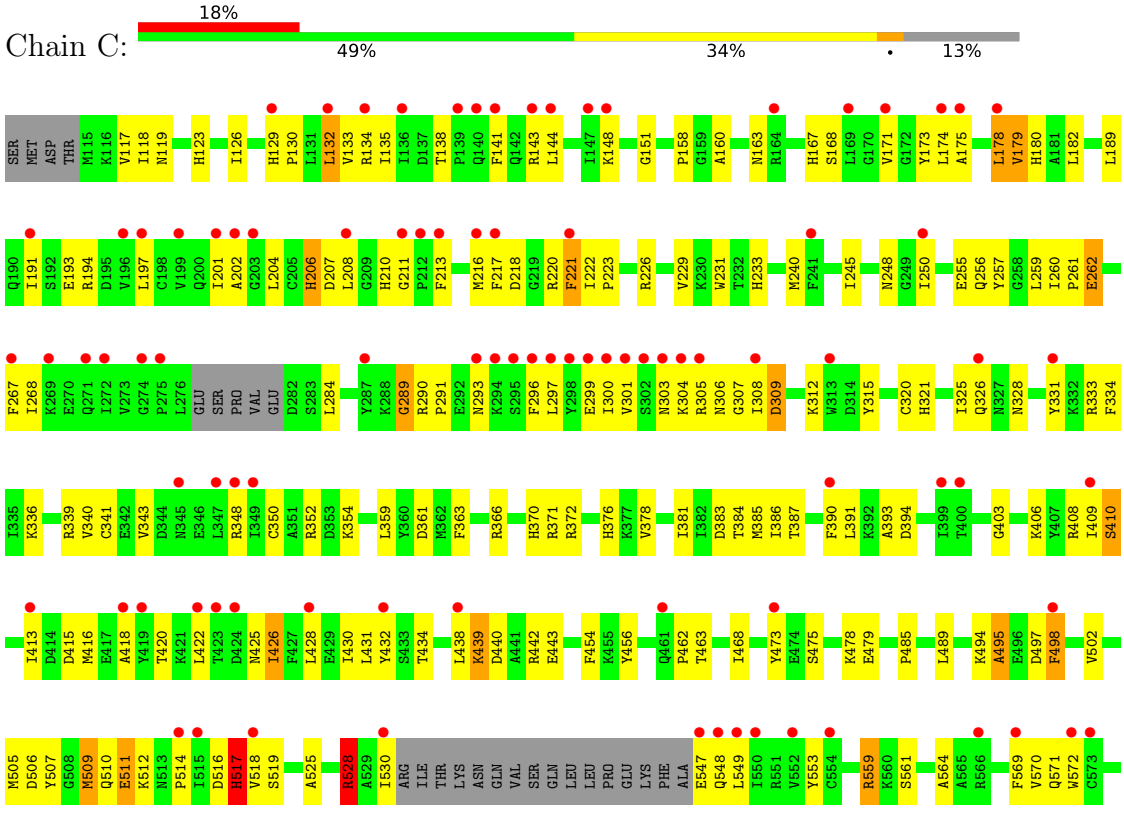
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

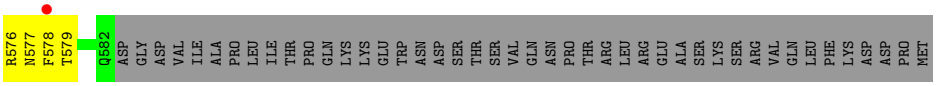
Chain B:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:




R576
N577
F578
T579
Q582
ASP GLY ASP VAL ILE ALA PRO LEU ILE THR PRO GLN LYS LYS GLU TRP ASN ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP PRO MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	202.57Å 81.88Å 154.03Å 90.00° 118.52° 90.00°	Depositor
Resolution (Å)	27.61 – 3.07 135.34 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.61-3.07) 99.6 (135.34-2.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.197 , 0.250 0.212 , 0.264	Depositor DCC
R_{free} test set	2864 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 86.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28956	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.67	0/3708	0.84	3/5001 (0.1%)
1	B	0.49	1/3698 (0.0%)	0.70	0/4987
1	C	0.46	1/3742 (0.0%)	0.69	0/5047
1	D	0.65	0/3720	0.85	4/5017 (0.1%)
All	All	0.58	2/14868 (0.0%)	0.77	7/20052 (0.0%)

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	10
1	B	0	9
1	C	0	9
1	D	0	10
All	All	0	38

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	CYS	CB-SG	-6.65	1.71	1.82
1	C	320	CYS	CB-SG	-6.01	1.72	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	ASP	CB-CG-OD2	10.57	127.82	118.30
1	A	314	ASP	CB-CG-OD1	8.51	125.96	118.30
1	D	120	ASP	CB-CG-OD2	-7.31	111.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	TYR	CA-CB-CG	6.00	124.80	113.40
1	D	311	ASP	OD1-CG-OD2	-5.75	112.37	123.30
1	A	315	TYR	CA-CB-CG	5.45	123.76	113.40
1	A	501	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	305	ARG	Sidechain
1	A	333	ARG	Sidechain
1	A	366	ARG	Sidechain
1	A	371	ARG	Sidechain
1	A	451	ARG	Sidechain
1	A	528	ARG	Sidechain
1	A	559	ARG	Sidechain
1	A	576	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	164	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	290	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	333	ARG	Sidechain
1	B	372	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	576	ARG	Sidechain
1	C	143	ARG	Sidechain
1	C	339	ARG	Sidechain
1	C	352	ARG	Sidechain
1	C	371	ARG	Sidechain
1	C	372	ARG	Sidechain
1	C	408	ARG	Sidechain
1	C	528	ARG	Sidechain
1	C	559	ARG	Sidechain
1	C	576	ARG	Sidechain
1	D	134	ARG	Sidechain
1	D	305	ARG	Sidechain
1	D	318	ARG	Sidechain
1	D	372	ARG	Sidechain
1	D	442	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	451	ARG	Sidechain
1	D	470	ARG	Sidechain
1	D	528	ARG	Sidechain
1	D	551	ARG	Sidechain
1	D	576	ARG	Sidechain

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	3623	3601	3601	68	1
1	B	3614	3589	3589	96	1
1	C	3656	3625	3625	151	1
1	D	3636	3607	3607	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	1	0
All	All	14534	14422	14422	368	2

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 13.

All (368) 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:242:GLU:OE1	1:A:269:LYS:NZ	2.00	0.94
1:A:513:ASN:ND2	1:A:516:ASP:OD2	2.01	0.94
1:B:428:LEU:HD13	1:C:425:ASN:HB3	1.52	0.89
1:C:134:ARG:NH2	1:C:250:ILE:HD13	1.88	0.88
1:D:220:ARG:HG2	1:D:387:THR:HG21	1.55	0.87
1:A:570:VAL:HG22	1:A:581:PRO:HG2	1.62	0.82
1:B:490:ASP:O	1:B:491:VAL:HG23	1.81	0.81
1:C:359:LEU:HD11	1:C:518:VAL:HG21	1.68	0.75
1:B:218:ASP:O	1:B:470:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:HIS:NE2	1:B:311:ASP:OD1	2.21	0.73
1:C:226:ARG:CZ	1:C:229:VAL:HG21	2.19	0.73
1:C:193:GLU:O	1:C:197:LEU:HD12	1.89	0.72
1:C:468:ILE:HD11	1:C:578:PHE:CZ	2.24	0.72
1:B:179:VAL:HG23	1:B:196:VAL:HG22	1.72	0.70
1:A:179:VAL:CG1	1:A:300:ILE:HD13	2.21	0.70
1:C:473:TYR:CE1	1:C:502:VAL:HG21	2.27	0.69
1:C:134:ARG:HH21	1:C:250:ILE:HD13	1.55	0.69
1:B:194:ARG:CZ	1:B:260:ILE:HD12	2.24	0.68
1:C:206:HIS:CD2	1:C:207:ASP:H	2.12	0.68
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.76	0.67
1:C:194:ARG:NH2	1:C:260:ILE:HD12	2.10	0.67
1:C:240:MET:SD	1:C:420:THR:HG22	2.36	0.66
1:C:267:PHE:HB2	1:C:289:GLY:HA3	1.77	0.65
1:C:168:SER:HB3	1:C:206:HIS:CD2	2.32	0.65
1:D:283:SER:O	1:D:284:LEU:HD23	1.96	0.64
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.77	0.64
1:B:118:ILE:HD12	1:B:128:LEU:HD12	1.79	0.64
1:C:507:TYR:CG	1:C:507:TYR:O	2.51	0.64
1:B:238:VAL:HG13	1:B:269:LYS:HG2	1.79	0.63
1:D:397:ILE:HG21	1:D:426:ILE:HD11	1.80	0.63
1:A:179:VAL:HG12	1:A:300:ILE:CD1	2.29	0.63
1:C:179:VAL:HG23	1:C:180:HIS:H	1.64	0.63
1:C:306:ASN:HB2	1:C:517:HIS:HB3	1.81	0.62
1:C:363:PHE:CD2	1:C:514:PRO:HB2	2.34	0.62
1:C:359:LEU:CD1	1:C:518:VAL:HG21	2.28	0.62
1:D:505:MET:O	1:D:547:GLU:HG2	1.98	0.61
1:C:222:ILE:HB	1:C:223:PRO:HD3	1.82	0.61
1:B:566:ARG:O	1:B:570:VAL:HG23	2.00	0.61
1:D:356:VAL:HG23	1:D:515:ILE:HG12	1.82	0.61
1:D:528:ARG:HH22	1:D:530:ILE:HG22	1.66	0.60
1:A:189:LEU:HD22	1:A:296:PHE:CE2	2.35	0.60
1:B:167:HIS:O	1:B:171:VAL:HG23	2.01	0.60
1:B:206:HIS:CD2	1:B:311:ASP:OD1	2.55	0.60
1:A:427:PHE:CE2	1:A:445:LEU:HD22	2.36	0.59
1:C:132:LEU:HD23	1:C:204:LEU:HD22	1.84	0.59
1:C:134:ARG:CZ	1:C:250:ILE:HD13	2.32	0.59
1:D:468:ILE:HG21	1:D:476:LEU:HD11	1.83	0.59
1:A:182:LEU:HD22	1:A:340:VAL:HG23	1.83	0.59
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.37	0.59
1:C:497:ASP:O	1:C:498:PHE:CD2	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG12	1:A:300:ILE:HD13	1.84	0.59
1:D:220:ARG:CG	1:D:387:THR:HG21	2.30	0.58
1:A:132:LEU:HB3	1:A:204:LEU:HD11	1.84	0.58
1:D:455:LYS:CG	1:D:557:VAL:HG12	2.32	0.58
1:B:468:ILE:HG21	1:B:476:LEU:HD11	1.86	0.58
1:D:309:ASP:OD2	1:D:312:LYS:HG2	2.03	0.58
1:B:570:VAL:HG22	1:B:581:PRO:HG2	1.85	0.57
1:B:136:ILE:HD11	1:B:204:LEU:HD21	1.86	0.57
1:C:366:ARG:HD3	1:C:509:MET:SD	2.45	0.57
1:C:118:ILE:HG23	1:C:119:ASN:N	2.19	0.57
1:B:129:HIS:CD2	1:B:130:PRO:HD2	2.40	0.56
1:D:283:SER:C	1:D:284:LEU:HD23	2.26	0.56
1:C:475:SER:HA	1:C:478:LYS:HE3	1.87	0.56
1:B:180:HIS:O	1:B:184:GLU:HG2	2.06	0.56
1:B:576:ARG:HH11	1:B:576:ARG:HB3	1.71	0.56
1:C:179:VAL:HG13	1:C:300:ILE:HD13	1.87	0.55
1:C:387:THR:HG22	1:C:391:LEU:HD11	1.88	0.55
1:C:510:GLN:O	1:C:511:GLU:C	2.45	0.55
1:C:217:PHE:CZ	1:C:222:ILE:HD11	2.41	0.55
1:A:455:LYS:CG	1:A:557:VAL:HG12	2.37	0.55
1:B:515:ILE:HD11	1:B:520:PHE:HZ	1.71	0.55
1:C:363:PHE:CE2	1:C:514:PRO:HB2	2.43	0.55
1:C:226:ARG:HH11	1:C:413:ILE:HD11	1.72	0.54
1:B:194:ARG:NH1	1:B:260:ILE:HD12	2.22	0.54
1:D:194:ARG:NH2	1:D:260:ILE:HD12	2.22	0.54
1:C:132:LEU:HA	1:C:135:ILE:HD12	1.89	0.54
1:D:467:LYS:HE3	1:D:547:GLU:HB3	1.89	0.54
1:D:495:ALA:O	1:D:497:ASP:N	2.41	0.54
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.88	0.54
1:A:416:MET:HG2	3:A:801:HOH:O	2.06	0.54
1:B:179:VAL:CG1	1:B:300:ILE:HD13	2.37	0.54
1:C:306:ASN:CB	1:C:517:HIS:HB3	2.38	0.54
1:C:284:LEU:O	1:C:284:LEU:HD23	2.08	0.54
1:D:495:ALA:O	1:D:498:PHE:N	2.24	0.54
1:C:189:LEU:HD22	1:C:296:PHE:CE1	2.42	0.53
1:B:189:LEU:HD22	1:B:296:PHE:CE2	2.44	0.53
1:C:182:LEU:HD22	1:C:340:VAL:HG23	1.90	0.53
1:B:226:ARG:NH1	1:B:413:ILE:HD11	2.24	0.53
1:B:148:LYS:HA	1:B:163:ASN:HA	1.91	0.53
1:C:202:ALA:HA	1:C:268:ILE:HG23	1.90	0.52
1:A:377:LYS:HD2	1:A:456:TYR:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:CG2	1:B:196:VAL:HG22	2.40	0.52
1:B:476:LEU:HD22	1:B:576:ARG:HH21	1.74	0.52
1:A:427:PHE:CZ	1:A:445:LEU:HD22	2.44	0.52
1:C:528:ARG:HH22	1:C:530:ILE:HG13	1.74	0.52
1:C:197:LEU:O	1:C:201:ILE:HD12	2.09	0.52
1:D:455:LYS:HG3	1:D:557:VAL:HG12	1.92	0.52
1:B:223:PRO:HB3	1:B:470:ARG:HB3	1.91	0.52
1:A:522:CYS:HB3	1:A:528:ARG:HH12	1.74	0.52
1:D:494:LYS:HD3	1:D:496:GLU:H	1.76	0.51
1:A:186:GLN:HB2	1:A:189:LEU:HD12	1.92	0.51
1:B:219:GLY:HA2	1:B:470:ARG:HH21	1.76	0.51
1:B:402:ALA:N	1:B:415:ASP:OD2	2.43	0.51
1:C:118:ILE:HG22	1:C:126:ILE:HB	1.92	0.51
1:A:329:PHE:CD1	1:A:362:MET:HB2	2.46	0.51
1:C:325:ILE:HG22	1:C:326:GLN:N	2.25	0.51
1:C:144:LEU:HD11	1:C:208:LEU:HD23	1.93	0.51
1:C:197:LEU:HB2	1:C:259:LEU:HD11	1.92	0.51
1:B:179:VAL:HG12	1:B:300:ILE:HD13	1.93	0.51
1:B:582:GLN:O	1:B:582:GLN:HG2	2.11	0.51
1:A:467:LYS:NZ	1:A:547:GLU:HB3	2.24	0.51
1:B:206:HIS:NE2	1:B:311:ASP:CG	2.64	0.51
1:D:120:ASP:HB2	1:D:126:ILE:HD12	1.93	0.51
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.94	0.51
1:D:141:PHE:HA	1:D:208:LEU:HD21	1.92	0.50
1:C:387:THR:O	1:C:391:LEU:HD12	2.11	0.50
1:D:528:ARG:NH2	1:D:530:ILE:HA	2.27	0.50
1:A:222:ILE:HB	1:A:223:PRO:HD3	1.94	0.49
1:A:484:LYS:O	1:A:485:PRO:C	2.51	0.49
1:A:340:VAL:HG13	1:A:348:ARG:O	2.12	0.49
1:C:226:ARG:HD2	1:C:410:SER:O	2.11	0.49
1:C:144:LEU:HD21	1:C:208:LEU:HA	1.95	0.49
1:C:475:SER:O	1:C:479:GLU:HG3	2.12	0.49
1:D:179:VAL:HG23	1:D:180:HIS:N	2.27	0.49
1:B:457:VAL:HB	1:B:552:VAL:O	2.12	0.49
1:C:390:PHE:CZ	1:C:426:ILE:HG23	2.48	0.49
1:C:231:TRP:CZ3	1:C:413:ILE:HB	2.47	0.49
1:D:167:HIS:CE1	1:D:315:TYR:HB3	2.48	0.49
1:B:205:CYS:HB3	1:B:208:LEU:HD12	1.95	0.49
1:C:129:HIS:ND1	1:C:197:LEU:HD21	2.28	0.49
1:C:409:ILE:HG23	1:C:422:LEU:HD11	1.95	0.49
1:C:216:MET:O	1:C:220:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLY:O	1:D:206:HIS:CD2	2.65	0.48
1:C:129:HIS:CG	1:C:197:LEU:HD21	2.48	0.48
1:C:385:MET:HG3	1:C:454:PHE:CD2	2.48	0.48
1:D:505:MET:O	1:D:547:GLU:CG	2.61	0.48
1:B:488:LEU:HD12	1:B:492:LYS:NZ	2.28	0.48
1:B:580:LYS:HG2	1:B:581:PRO:HD2	1.95	0.48
1:C:134:ARG:HH21	1:C:250:ILE:CD1	2.23	0.48
1:C:343:VAL:HB	1:C:348:ARG:HG3	1.95	0.48
1:B:515:ILE:HD11	1:B:520:PHE:CZ	2.47	0.48
1:C:393:ALA:HB1	1:C:438:LEU:HD22	1.95	0.48
1:C:473:TYR:CZ	1:C:502:VAL:HG21	2.48	0.48
1:B:489:LEU:N	1:B:489:LEU:HD22	2.29	0.48
1:C:141:PHE:CD1	1:C:208:LEU:HD21	2.49	0.48
1:C:245:ILE:HG22	1:C:250:ILE:HB	1.95	0.48
1:B:428:LEU:CD1	1:C:425:ASN:HB3	2.35	0.48
1:C:312:LYS:HA	1:C:315:TYR:HD2	1.79	0.48
1:D:264:ASP:O	1:D:268:ILE:HD12	2.14	0.47
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.49	0.47
1:B:334:PHE:O	1:B:338:ALA:HB2	2.14	0.47
1:A:189:LEU:HD22	1:A:296:PHE:CZ	2.49	0.47
1:C:126:ILE:HG23	1:C:173:TYR:CD2	2.49	0.47
1:C:126:ILE:HG23	1:C:173:TYR:HD2	1.79	0.47
1:D:203:GLY:O	1:D:206:HIS:HD2	1.96	0.47
1:C:206:HIS:CG	1:C:207:ASP:N	2.83	0.47
1:C:561:SER:O	1:C:564:ALA:HB3	2.13	0.47
1:D:425:ASN:ND2	1:A:425:ASN:OD1	2.47	0.47
1:A:478:LYS:HA	1:A:495:ALA:HB2	1.97	0.47
1:C:130:PRO:O	1:C:133:VAL:HB	2.14	0.47
1:C:431:LEU:HD23	1:C:432:TYR:CE1	2.49	0.47
1:B:575:ASP:OD1	1:B:575:ASP:O	2.33	0.47
1:C:218:ASP:OD2	1:C:233:HIS:HB3	2.14	0.47
1:A:428:LEU:HD22	1:A:432:TYR:CZ	2.50	0.47
1:C:189:LEU:HD13	1:C:191:ILE:HD11	1.97	0.47
1:A:576:ARG:HD3	1:A:578:PHE:CE2	2.50	0.47
1:B:245:ILE:HG13	1:B:246:ASN:N	2.30	0.47
1:B:393:ALA:HB1	1:B:438:LEU:CD2	2.45	0.47
1:A:356:VAL:HG13	1:A:357:GLY:N	2.30	0.46
1:C:179:VAL:HG23	1:C:180:HIS:N	2.30	0.46
1:D:467:LYS:CE	1:D:547:GLU:HB3	2.46	0.46
1:C:385:MET:HG3	1:C:454:PHE:CE2	2.50	0.46
1:C:178:LEU:O	1:C:179:VAL:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ILE:HG23	1:A:454:PHE:HB2	1.96	0.46
1:B:179:VAL:HG12	1:B:300:ILE:CD1	2.46	0.46
1:C:525:ALA:HB1	1:C:528:ARG:CG	2.46	0.46
1:A:179:VAL:HG23	1:A:180:HIS:N	2.29	0.46
1:C:299:GLU:OE1	1:C:305:ARG:NH2	2.49	0.46
1:C:505:MET:HG2	1:C:547:GLU:O	2.15	0.46
1:D:399:ILE:CD1	1:D:422:LEU:HD13	2.45	0.46
1:B:353:ASP:OD1	1:B:353:ASP:N	2.47	0.46
1:C:301:VAL:HG12	1:C:301:VAL:O	2.15	0.46
1:D:497:ASP:OD1	1:D:556:LYS:HE2	2.15	0.46
1:A:468:ILE:HG21	1:A:476:LEU:HD11	1.97	0.46
1:C:167:HIS:O	1:C:171:VAL:HG23	2.15	0.46
1:D:123:HIS:HB3	1:D:173:TYR:CE2	2.51	0.45
1:B:433:SER:HB2	1:B:438:LEU:HD12	1.99	0.45
1:B:465:GLN:O	1:B:466:ILE:C	2.54	0.45
1:B:493:LEU:HD12	1:B:568:TYR:HD2	1.81	0.45
1:D:300:ILE:O	1:D:310:VAL:HG22	2.16	0.45
1:B:166:GLU:O	1:B:167:HIS:C	2.55	0.45
1:C:376:HIS:CE1	1:C:378:VAL:HB	2.51	0.45
1:D:356:VAL:HG13	1:D:357:GLY:N	2.32	0.45
1:A:132:LEU:HD22	1:A:204:LEU:HD12	1.98	0.45
1:C:439:LYS:HE3	1:C:443:GLU:OE2	2.16	0.45
1:C:510:GLN:OE1	1:C:512:LYS:HG2	2.17	0.45
1:D:572:TRP:HA	1:D:575:ASP:OD1	2.16	0.45
1:A:525:ALA:HB3	1:A:528:ARG:HD3	1.99	0.45
1:D:206:HIS:ND1	1:D:207:ASP:OD1	2.41	0.45
1:C:175:ALA:O	1:C:179:VAL:HG22	2.17	0.45
1:C:303:ASN:C	1:C:305:ARG:H	2.18	0.45
1:C:462:PRO:HA	1:C:578:PHE:CD1	2.52	0.45
1:C:117:VAL:HG13	1:C:126:ILE:O	2.16	0.45
1:C:132:LEU:CD2	1:C:204:LEU:HD22	2.46	0.45
1:C:511:GLU:OE1	1:C:516:ASP:HB3	2.16	0.45
1:C:328:ASN:HB2	1:C:361:ASP:HB3	1.98	0.45
1:A:171:VAL:HG13	1:A:310:VAL:HG23	1.99	0.45
1:B:118:ILE:HD12	1:B:128:LEU:CD1	2.47	0.45
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.51	0.45
1:C:179:VAL:HG12	1:C:297:LEU:CD2	2.46	0.45
1:C:303:ASN:O	1:C:305:ARG:N	2.50	0.45
1:D:513:ASN:ND2	1:D:514:PRO:HD2	2.32	0.45
1:B:377:LYS:HD2	1:B:456:TYR:HB2	1.99	0.44
1:B:370:HIS:HA	1:B:374:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ARG:HD2	1:D:420:THR:HA	2.00	0.44
1:A:476:LEU:O	1:A:477:PRO:C	2.54	0.44
1:C:217:PHE:HA	1:C:221:PHE:HB3	1.99	0.44
1:C:301:VAL:O	1:C:301:VAL:CG1	2.65	0.44
1:B:557:VAL:HA	1:B:562:LEU:HD21	1.99	0.44
1:C:134:ARG:HE	1:C:250:ILE:HD11	1.83	0.44
1:C:370:HIS:CE1	1:C:509:MET:SD	3.11	0.44
1:C:430:ILE:HG22	1:C:430:ILE:O	2.17	0.44
1:D:455:LYS:HG2	1:D:557:VAL:HG12	1.98	0.44
1:C:384:THR:HG21	1:C:553:TYR:HE2	1.83	0.44
1:B:466:ILE:HG23	1:B:466:ILE:O	2.17	0.44
1:C:261:PRO:O	1:C:262:GLU:C	2.55	0.44
1:C:303:ASN:H	1:C:309:ASP:HB3	1.81	0.44
1:A:166:GLU:OE1	1:A:166:GLU:N	2.38	0.44
1:B:552:VAL:HB	1:B:569:PHE:CD1	2.52	0.44
1:C:290:ARG:HB3	1:C:291:PRO:HD2	2.00	0.44
1:C:468:ILE:HD11	1:C:578:PHE:HZ	1.76	0.44
1:B:402:ALA:HB2	1:B:415:ASP:OD1	2.18	0.44
1:C:222:ILE:HG21	1:C:231:TRP:HB3	2.00	0.44
1:A:115:MET:O	1:A:116:LYS:HB2	2.18	0.44
1:C:394:ASP:HA	1:C:409:ILE:HD12	2.00	0.44
1:D:249:GLY:O	1:D:252:PRO:HD2	2.17	0.43
1:A:453:LEU:N	1:A:453:LEU:HD23	2.32	0.43
1:A:123:HIS:HE1	1:A:174:LEU:HD11	1.83	0.43
1:A:167:HIS:O	1:A:171:VAL:HG23	2.18	0.43
1:B:352:ARG:HG2	1:B:353:ASP:OD1	2.18	0.43
1:B:448:ILE:HA	1:B:453:LEU:CD2	2.48	0.43
1:C:178:LEU:HD23	1:C:300:ILE:HG23	2.00	0.43
1:C:416:MET:O	1:C:420:THR:CG2	2.66	0.43
1:A:179:VAL:HG23	1:A:196:VAL:HG22	2.01	0.43
1:A:194:ARG:NH2	1:A:260:ILE:HD12	2.32	0.43
1:A:229:VAL:HG12	1:A:230:LYS:N	2.34	0.43
1:A:480:VAL:HG11	1:A:498:PHE:CD1	2.53	0.43
1:B:229:VAL:HG12	1:B:230:LYS:N	2.32	0.43
1:B:259:LEU:N	1:B:259:LEU:HD12	2.34	0.43
1:B:390:PHE:CZ	1:B:426:ILE:HG21	2.54	0.43
1:C:213:PHE:CE2	1:C:386:ILE:HD13	2.53	0.43
1:C:333:ARG:O	1:C:336:LYS:HG2	2.17	0.43
1:C:463:THR:HG23	1:C:579:THR:HG23	2.00	0.43
1:D:444:ILE:O	1:D:447:GLN:HB2	2.19	0.43
1:D:339:ARG:HB2	1:D:521:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:N	1:D:223:PRO:CD	2.81	0.43
1:A:157:PHE:CG	1:A:323:LEU:CD2	3.01	0.43
1:A:157:PHE:CG	1:A:323:LEU:HD23	2.53	0.43
1:A:364:HIS:CE1	1:B:354:LYS:HG2	2.54	0.43
1:D:462:PRO:HG3	1:D:550:ILE:HD11	2.00	0.43
1:B:575:ASP:OD1	1:B:575:ASP:C	2.56	0.43
1:C:509:MET:HE3	1:C:509:MET:HB2	1.69	0.43
1:D:131:LEU:HD13	1:D:253:VAL:HG12	2.00	0.43
1:D:399:ILE:HD11	1:D:422:LEU:HD13	2.01	0.43
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.43
1:C:148:LYS:HA	1:C:163:ASN:HA	2.00	0.43
1:C:206:HIS:CD2	1:C:207:ASP:N	2.84	0.43
1:C:303:ASN:C	1:C:305:ARG:N	2.72	0.43
1:C:333:ARG:O	1:C:334:PHE:C	2.57	0.43
1:C:381:ILE:HD11	1:C:456:TYR:HB2	2.00	0.43
1:D:457:VAL:HB	1:D:552:VAL:O	2.19	0.43
1:A:566:ARG:O	1:A:570:VAL:HG23	2.19	0.43
1:C:307:GLY:O	1:C:312:LYS:HD2	2.19	0.43
1:D:114:THR:O	1:D:115:MET:C	2.58	0.42
1:B:220:ARG:NH2	1:B:387:THR:HB	2.33	0.42
1:C:174:LEU:CD2	1:C:331:TYR:CE2	3.02	0.42
1:C:428:LEU:HD22	1:C:432:TYR:CE2	2.54	0.42
1:B:119:ASN:O	1:C:158:PRO:HD2	2.19	0.42
1:B:141:PHE:HA	1:B:208:LEU:HD21	2.00	0.42
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.01	0.42
1:C:485:PRO:HB2	1:C:489:LEU:HD23	2.01	0.42
1:A:123:HIS:CE1	1:A:174:LEU:HD11	2.54	0.42
1:A:260:ILE:O	1:A:261:PRO:C	2.58	0.42
1:B:143:ARG:NH2	1:B:210:HIS:O	2.51	0.42
1:B:245:ILE:HA	1:B:250:ILE:CG1	2.50	0.42
1:C:394:ASP:CA	1:C:409:ILE:HD12	2.49	0.42
1:C:548:GLN:O	1:C:549:LEU:HD22	2.19	0.42
1:D:186:GLN:HB2	1:D:189:LEU:HD12	2.01	0.42
1:D:515:ILE:HD11	1:D:520:PHE:HZ	1.83	0.42
1:A:334:PHE:O	1:A:338:ALA:HB2	2.20	0.42
1:B:325:ILE:HG22	1:B:326:GLN:N	2.35	0.42
1:C:439:LYS:O	1:C:442:ARG:N	2.52	0.42
1:B:182:LEU:HD22	1:B:340:VAL:HG23	2.01	0.42
1:B:194:ARG:HD2	1:B:258:GLY:O	2.19	0.42
1:B:400:THR:OG1	1:C:434:THR:HG21	2.19	0.42
1:C:439:LYS:O	1:C:440:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLU:HB3	1:A:158:PRO:O	2.19	0.42
1:D:474:GLU:O	1:D:477:PRO:HD2	2.19	0.42
1:B:215:HIS:O	1:B:216:MET:C	2.56	0.42
1:C:343:VAL:HG21	1:C:348:ARG:HB2	2.01	0.42
1:C:494:LYS:HG2	1:C:495:ALA:H	1.84	0.42
1:C:255:GLU:HG2	1:C:261:PRO:CD	2.49	0.42
1:C:528:ARG:NH2	1:C:530:ILE:HG13	2.35	0.42
1:A:174:LEU:HD21	1:A:331:TYR:CZ	2.55	0.42
1:B:483:ALA:HB3	1:B:568:TYR:HD1	1.85	0.42
1:C:144:LEU:HD11	1:C:208:LEU:CD2	2.48	0.42
1:C:211:GLY:HA3	1:C:217:PHE:HB3	2.01	0.42
1:A:211:GLY:O	1:A:212:PRO:C	2.58	0.42
1:B:365:THR:O	1:B:366:ARG:C	2.56	0.42
1:D:238:VAL:HG13	1:D:269:LYS:HG2	2.01	0.41
1:A:167:HIS:HD2	1:A:171:VAL:HG23	1.84	0.41
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.82	0.41
1:B:250:ILE:HG22	1:B:254:MET:HG3	2.01	0.41
1:B:141:PHE:O	1:B:143:ARG:N	2.53	0.41
1:B:433:SER:OG	1:B:442:ARG:NH1	2.51	0.41
1:C:428:LEU:HD23	1:C:428:LEU:HA	1.92	0.41
1:C:569:PHE:O	1:C:570:VAL:C	2.58	0.41
1:A:467:LYS:HZ3	1:A:547:GLU:HB3	1.83	0.41
1:B:321:HIS:CD2	1:C:321:HIS:CE1	3.07	0.41
1:B:490:ASP:O	1:B:491:VAL:CG2	2.60	0.41
1:D:428:LEU:HD11	1:A:146:TYR:CD1	2.56	0.41
1:C:138:THR:HB	1:C:248:ASN:ND2	2.35	0.41
1:C:179:VAL:O	1:C:180:HIS:C	2.58	0.41
1:C:366:ARG:CD	1:C:509:MET:SD	3.08	0.41
1:B:393:ALA:HB1	1:B:438:LEU:HD22	2.02	0.41
1:C:217:PHE:HA	1:C:221:PHE:CB	2.51	0.41
1:C:409:ILE:CD1	1:C:426:ILE:HD11	2.51	0.41
1:D:223:PRO:HG2	1:D:470:ARG:HD3	2.03	0.41
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.20	0.41
1:A:179:VAL:HG12	1:A:300:ILE:HD11	2.00	0.41
1:C:226:ARG:NH2	1:C:229:VAL:HG21	2.35	0.41
1:C:256:GLN:OE1	1:C:257:TYR:CD2	2.74	0.41
1:D:218:ASP:O	1:D:470:ARG:NH1	2.53	0.41
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.02	0.41
1:A:167:HIS:CD2	1:A:171:VAL:HG23	2.56	0.41
1:A:360:TYR:CD2	1:B:356:VAL:HG11	2.55	0.41
1:C:571:GLN:O	1:C:572:TRP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLN:OE1	1:D:164:ARG:NH1	2.54	0.41
1:D:251:LYS:CB	1:D:252:PRO:HD3	2.51	0.41
1:B:407:TYR:CZ	1:B:415:ASP:HB2	2.56	0.41
1:B:485:PRO:HG3	1:B:489:LEU:HD21	2.03	0.41
1:B:488:LEU:N	1:B:488:LEU:HD22	2.35	0.41
1:C:394:ASP:OD1	1:C:409:ILE:N	2.54	0.41
1:D:495:ALA:O	1:D:496:GLU:C	2.58	0.41
1:A:513:ASN:OD1	1:A:513:ASN:N	2.46	0.41
1:A:563:TYR:O	1:A:567:GLN:HG2	2.21	0.41
1:B:339:ARG:HD3	1:B:521:TYR:CZ	2.56	0.41
1:B:433:SER:CB	1:B:438:LEU:HD12	2.50	0.41
1:C:210:HIS:HA	1:C:233:HIS:HB2	2.03	0.41
1:C:439:LYS:HD3	1:C:442:ARG:HH21	1.86	0.41
1:C:506:ASP:OD1	1:C:506:ASP:C	2.58	0.41
1:D:215:HIS:O	1:D:216:MET:C	2.55	0.41
1:C:385:MET:HG2	1:C:454:PHE:CZ	2.56	0.41
1:D:321:HIS:CE1	1:A:321:HIS:CE1	3.09	0.40
1:B:301:VAL:O	1:B:309:ASP:HB2	2.21	0.40
1:B:350:CYS:HB3	1:B:519:SER:C	2.42	0.40
1:B:556:LYS:O	1:B:562:LEU:HD21	2.22	0.40
1:C:226:ARG:NH1	1:C:413:ILE:HD11	2.35	0.40
1:C:415:ASP:HB3	1:C:418:ALA:HB3	2.03	0.40
1:D:171:VAL:HG22	1:D:311:ASP:HA	2.03	0.40
1:A:205:CYS:HB3	1:A:208:LEU:HD12	2.04	0.40
1:C:220:ARG:HG2	1:C:387:THR:HG21	2.03	0.40
1:C:428:LEU:HD22	1:C:432:TYR:CZ	2.55	0.40
1:C:494:LYS:O	1:C:497:ASP:N	2.53	0.40
1:D:223:PRO:CG	1:D:470:ARG:HD3	2.51	0.40
1:D:495:ALA:C	1:D:497:ASP:N	2.75	0.40
1:B:466:ILE:O	1:B:466:ILE:CG2	2.70	0.40
1:C:291:PRO:CG	1:C:293:ASN:OD1	2.69	0.40

All (2) 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:344:ASP:O	1:C:577:ASN:ND2[1_545]	1.93	0.27
1:A:262:GLU:OE2	1:A:262:GLU:OE2[2_555]	2.13	0.07

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	435/516 (84%)	397 (91%)	33 (8%)	5 (1%)	14 44
1	B	434/516 (84%)	385 (89%)	38 (9%)	11 (2%)	5 25
1	C	441/516 (86%)	351 (80%)	70 (16%)	20 (4%)	2 13
1	D	437/516 (85%)	409 (94%)	24 (6%)	4 (1%)	17 49
All	All	1747/2064 (85%)	1542 (88%)	165 (9%)	40 (2%)	6 26

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	491	VAL
1	C	439	LYS
1	C	498	PHE
1	C	517	HIS
1	D	496	GLU
1	D	514	PRO
1	A	116	LYS
1	A	151	GLY
1	B	466	ILE
1	C	160	ALA
1	C	262	GLU
1	C	308	ILE
1	C	511	GLU
1	D	115	MET
1	A	262	GLU
1	B	409	ILE
1	B	454	PHE
1	B	514	PRO
1	C	304	LYS
1	C	495	ALA
1	C	509	MET
1	B	221	PHE

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Mol	Chain	Res	Type
1	B	526	PRO
1	C	151	GLY
1	C	221	PHE
1	C	403	GLY
1	C	410	SER
1	B	142	GLN
1	B	206	HIS
1	B	212	PRO
1	C	123	HIS
1	C	178	LEU
1	C	519	SER
1	D	305	ARG
1	A	462	PRO
1	B	283	SER
1	C	179	VAL
1	C	426	ILE
1	A	261	PRO
1	C	289	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	392/461 (85%)	386 (98%)	6 (2%)	65	84
1	B	392/461 (85%)	385 (98%)	7 (2%)	59	80
1	C	396/461 (86%)	385 (97%)	11 (3%)	43	71
1	D	395/461 (86%)	390 (99%)	5 (1%)	69	86
All	All	1575/1844 (85%)	1546 (98%)	29 (2%)	59	80

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	309	ASP
1	D	315	TYR
1	D	341	CYS

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Mol	Chain	Res	Type
1	D	440	ASP
1	D	580	LYS
1	A	134	ARG
1	A	143	ARG
1	A	341	CYS
1	A	350	CYS
1	A	366	ARG
1	A	475	SER
1	B	341	CYS
1	B	350	CYS
1	B	370	HIS
1	B	419	TYR
1	B	435	ASP
1	B	497	ASP
1	B	506	ASP
1	C	132	LEU
1	C	206	HIS
1	C	309	ASP
1	C	341	CYS
1	C	350	CYS
1	C	354	LYS
1	C	383	ASP
1	C	406	LYS
1	C	517	HIS
1	C	528	ARG
1	C	559	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	322	HIS
1	A	321	HIS
1	A	364	HIS
1	A	527	ASN
1	B	322	HIS
1	B	447	GLN
1	C	140	GLN
1	C	248	ASN
1	C	322	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	443/516 (85%)	0.01	2 (0%) 91 80	57, 82, 145, 229	0
1	B	442/516 (85%)	0.54	58 (13%) 3 1	83, 139, 206, 241	0
1	C	447/516 (86%)	0.93	92 (20%) 1 0	96, 169, 221, 269	0
1	D	445/516 (86%)	0.06	3 (0%) 87 74	59, 85, 160, 233	0
All	All	1777/2064 (86%)	0.38	155 (8%) 10 3	57, 113, 205, 269	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	498	PHE	8.4
1	C	296	PHE	7.7
1	B	480	VAL	6.8
1	C	297	LEU	6.8
1	C	300	ILE	6.0
1	C	141	PHE	5.9
1	B	390	PHE	5.8
1	B	151	GLY	5.4
1	C	250	ILE	5.3
1	C	422	LEU	5.3
1	C	212	PRO	5.1
1	C	298	TYR	4.9
1	C	301	VAL	4.9
1	B	554	CYS	4.8
1	C	305	ARG	4.8
1	C	208	LEU	4.7
1	C	400	THR	4.6
1	B	501	ASP	4.5
1	C	390	PHE	4.5
1	B	473	TYR	4.5
1	C	144	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	178	LEU	4.4
1	C	203	GLY	4.3
1	C	303	ASN	4.2
1	C	413	ILE	4.2
1	C	424	ASP	4.2
1	C	241	PHE	4.1
1	C	140	GLN	4.1
1	C	554	CYS	4.0
1	C	550	ILE	4.0
1	C	132	LEU	3.9
1	C	409	ILE	3.9
1	C	347	LEU	3.8
1	C	217	PHE	3.8
1	B	382	ILE	3.7
1	C	191	ILE	3.7
1	C	572	TRP	3.7
1	C	518	VAL	3.7
1	B	572	TRP	3.6
1	B	556	LYS	3.6
1	C	148	LYS	3.6
1	C	201	ILE	3.6
1	C	294	LYS	3.5
1	C	136	ILE	3.5
1	C	418	ALA	3.5
1	C	399	ILE	3.5
1	C	171	VAL	3.4
1	C	271	GLN	3.4
1	C	295	SER	3.3
1	C	569	PHE	3.3
1	C	348	ARG	3.3
1	C	272	ILE	3.3
1	C	548	GLN	3.2
1	C	473	TYR	3.2
1	C	349	ILE	3.2
1	C	304	LYS	3.1
1	B	500	VAL	3.1
1	C	547	GLU	3.1
1	B	389	ALA	3.1
1	C	174	LEU	3.1
1	B	565	ALA	3.1
1	B	427	PHE	3.0
1	C	345	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	498	PHE	3.0
1	C	566	ARG	2.9
1	B	155	TYR	2.9
1	B	553	TYR	2.9
1	B	429	GLU	2.9
1	C	331	TYR	2.9
1	C	274	GLY	2.9
1	C	147	ILE	2.9
1	B	432	TYR	2.9
1	C	139	PRO	2.9
1	B	441	ALA	2.8
1	C	293	ASN	2.8
1	D	516	ASP	2.8
1	C	211	GLY	2.8
1	C	216	MET	2.8
1	B	208	LEU	2.8
1	C	175	ALA	2.8
1	C	423	THR	2.7
1	C	287	TYR	2.7
1	B	551	ARG	2.7
1	B	306	ASN	2.7
1	C	549	LEU	2.7
1	C	515	ILE	2.7
1	B	550	ILE	2.7
1	B	573	CYS	2.6
1	C	213	PHE	2.6
1	B	216	MET	2.6
1	C	461	GLN	2.6
1	C	196	VAL	2.6
1	B	220	ARG	2.6
1	A	343	VAL	2.5
1	C	275	PRO	2.5
1	B	450	TYR	2.5
1	B	455	LYS	2.5
1	B	438	LEU	2.5
1	D	527	ASN	2.5
1	C	269	LYS	2.5
1	B	515	ILE	2.5
1	B	213	PHE	2.5
1	C	432	TYR	2.4
1	B	499	ILE	2.4
1	B	445	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	419	TYR	2.4
1	B	549	LEU	2.4
1	C	578	PHE	2.4
1	B	409	ILE	2.4
1	B	428	LEU	2.4
1	C	169	LEU	2.4
1	B	578	PHE	2.4
1	C	326	GLN	2.3
1	B	337	PHE	2.3
1	B	561	SER	2.3
1	B	569	PHE	2.3
1	C	313	TRP	2.3
1	C	143	ARG	2.3
1	A	545	PHE	2.3
1	B	152	GLY	2.3
1	D	305	ARG	2.3
1	C	514	PRO	2.3
1	B	431	LEU	2.2
1	B	489	LEU	2.2
1	B	497	ASP	2.2
1	B	150	LEU	2.2
1	B	434	THR	2.2
1	C	302	SER	2.2
1	C	308	ILE	2.2
1	B	386	ILE	2.2
1	B	276	LEU	2.2
1	C	199	VAL	2.2
1	B	241	PHE	2.2
1	B	566	ARG	2.2
1	C	428	LEU	2.2
1	B	468	ILE	2.2
1	C	202	ALA	2.2
1	C	267	PHE	2.1
1	B	460	THR	2.1
1	C	129	HIS	2.1
1	C	221	PHE	2.1
1	C	438	LEU	2.1
1	C	134	ARG	2.1
1	C	530	ILE	2.1
1	C	164	ARG	2.1
1	C	299	GLU	2.1
1	B	217	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	422	LEU	2.1
1	B	323	LEU	2.1
1	B	397	ILE	2.1
1	C	573	CYS	2.0
1	B	530	ILE	2.0
1	C	552	VAL	2.0
1	C	197	LEU	2.0
1	B	221	PHE	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, 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	B-factors(Å^2)	Q<0.9
2	FE	D	701	1/1	0.01	0.52	201,201,201,201	0
2	FE	C	701	1/1	0.75	0.16	163,163,163,163	0
2	FE	A	701	1/1	0.87	0.27	76,76,76,76	0
2	FE	B	701	1/1	0.95	0.15	111,111,111,111	0

6.5 Other polymers (i)

There are no such residues in this entry.