Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 02:49 PM EDT

PDB ID	:	3QS9
Title	:	Crystal structure of a human Flt3 ligand-receptor ternary complex
Authors	:	Verstraete, K.; Savvides, S.N.
Deposited on	:	2011-02-20
Resolution	:	7.80 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 (i) 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 (1)) were used in the production of this report:

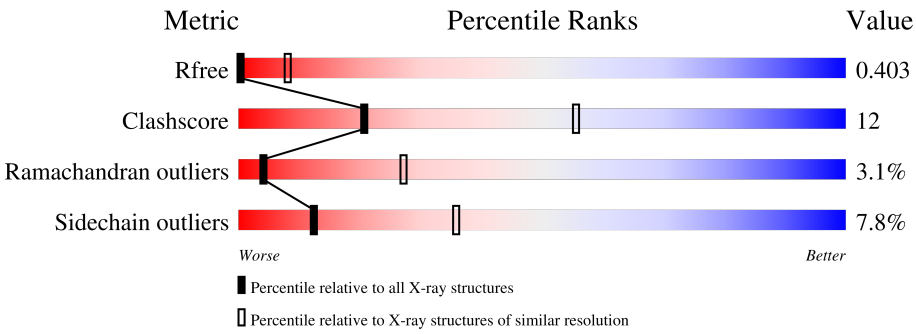
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 7.80 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	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	138	72% 20% • 6%
1	B	138	72% 19% • 6%
1	C	138	72% 19% • 6%
1	D	138	72% 19% • 6%
2	E	527	59% 16% • 23%
2	F	527	47% 14% • 38%
2	G	527	59% 17% • 23%

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Mol	Chain	Length	Quality of chain
2	H	527	59% 16% • 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13542 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 SL cytokine.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	130	1033	657	181	187	8	0	0	0
1	B	130	1033	657	181	187	8	0	0	0
1	C	130	1033	657	181	187	8	0	0	0
1	D	130	1033	657	181	187	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49771
A	-2	SER	-	expression tag	UNP P49771
A	-1	HIS	-	expression tag	UNP P49771
A	0	MET	-	expression tag	UNP P49771
B	-3	GLY	-	expression tag	UNP P49771
B	-2	SER	-	expression tag	UNP P49771
B	-1	HIS	-	expression tag	UNP P49771
B	0	MET	-	expression tag	UNP P49771
C	-3	GLY	-	expression tag	UNP P49771
C	-2	SER	-	expression tag	UNP P49771
C	-1	HIS	-	expression tag	UNP P49771
C	0	MET	-	expression tag	UNP P49771
D	-3	GLY	-	expression tag	UNP P49771
D	-2	SER	-	expression tag	UNP P49771
D	-1	HIS	-	expression tag	UNP P49771
D	0	MET	-	expression tag	UNP P49771

- Molecule 2 is a protein called FL cytokine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	405	2463	1586	427	433	17	0	0	0
2	F	329	2021	1301	350	355	15	0	0	0
2	G	405	2463	1586	427	433	17	0	0	0
2	H	405	2463	1586	427	433	17	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	24	GLU	-	expression tag	UNP P36888
E	25	THR	-	expression tag	UNP P36888
E	26	GLY	-	expression tag	UNP P36888
E	541	GLY	-	expression tag	UNP P36888
E	542	GLY	-	expression tag	UNP P36888
E	543	THR	-	expression tag	UNP P36888
E	544	LYS	-	expression tag	UNP P36888
E	545	HIS	-	expression tag	UNP P36888
E	546	HIS	-	expression tag	UNP P36888
E	547	HIS	-	expression tag	UNP P36888
E	548	HIS	-	expression tag	UNP P36888
E	549	HIS	-	expression tag	UNP P36888
E	550	HIS	-	expression tag	UNP P36888
F	24	GLU	-	expression tag	UNP P36888
F	25	THR	-	expression tag	UNP P36888
F	26	GLY	-	expression tag	UNP P36888
F	541	GLY	-	expression tag	UNP P36888
F	542	GLY	-	expression tag	UNP P36888
F	543	THR	-	expression tag	UNP P36888
F	544	LYS	-	expression tag	UNP P36888
F	545	HIS	-	expression tag	UNP P36888
F	546	HIS	-	expression tag	UNP P36888
F	547	HIS	-	expression tag	UNP P36888
F	548	HIS	-	expression tag	UNP P36888
F	549	HIS	-	expression tag	UNP P36888
F	550	HIS	-	expression tag	UNP P36888
G	24	GLU	-	expression tag	UNP P36888
G	25	THR	-	expression tag	UNP P36888
G	26	GLY	-	expression tag	UNP P36888
G	541	GLY	-	expression tag	UNP P36888
G	542	GLY	-	expression tag	UNP P36888

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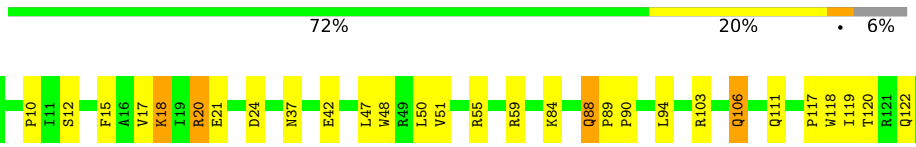
Chain	Residue	Modelled	Actual	Comment	Reference
G	543	THR	-	expression tag	UNP P36888
G	544	LYS	-	expression tag	UNP P36888
G	545	HIS	-	expression tag	UNP P36888
G	546	HIS	-	expression tag	UNP P36888
G	547	HIS	-	expression tag	UNP P36888
G	548	HIS	-	expression tag	UNP P36888
G	549	HIS	-	expression tag	UNP P36888
G	550	HIS	-	expression tag	UNP P36888
H	24	GLU	-	expression tag	UNP P36888
H	25	THR	-	expression tag	UNP P36888
H	26	GLY	-	expression tag	UNP P36888
H	541	GLY	-	expression tag	UNP P36888
H	542	GLY	-	expression tag	UNP P36888
H	543	THR	-	expression tag	UNP P36888
H	544	LYS	-	expression tag	UNP P36888
H	545	HIS	-	expression tag	UNP P36888
H	546	HIS	-	expression tag	UNP P36888
H	547	HIS	-	expression tag	UNP P36888
H	548	HIS	-	expression tag	UNP P36888
H	549	HIS	-	expression tag	UNP P36888
H	550	HIS	-	expression tag	UNP P36888

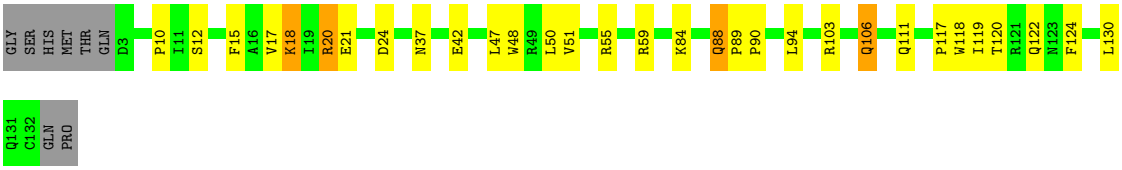
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SL cytokine

Chain A:



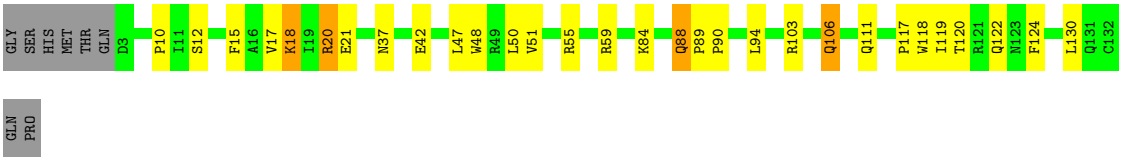


• Molecule 1: SL cytokine

Chain B:

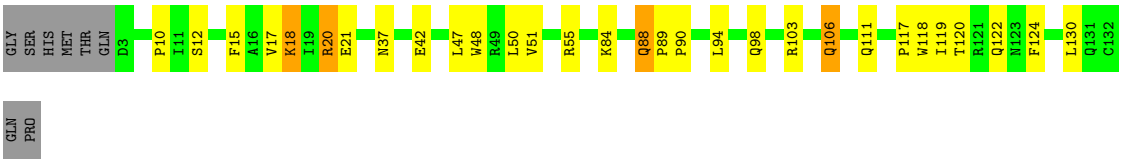
• Molecule 1: SL cytokine

Chain C:



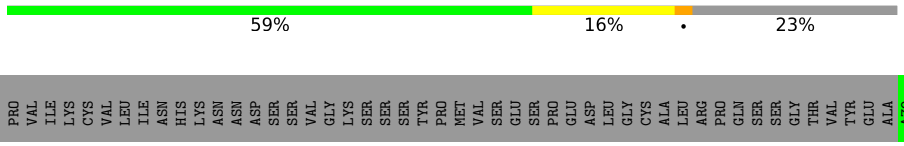
• Molecule 1: SL cytokine

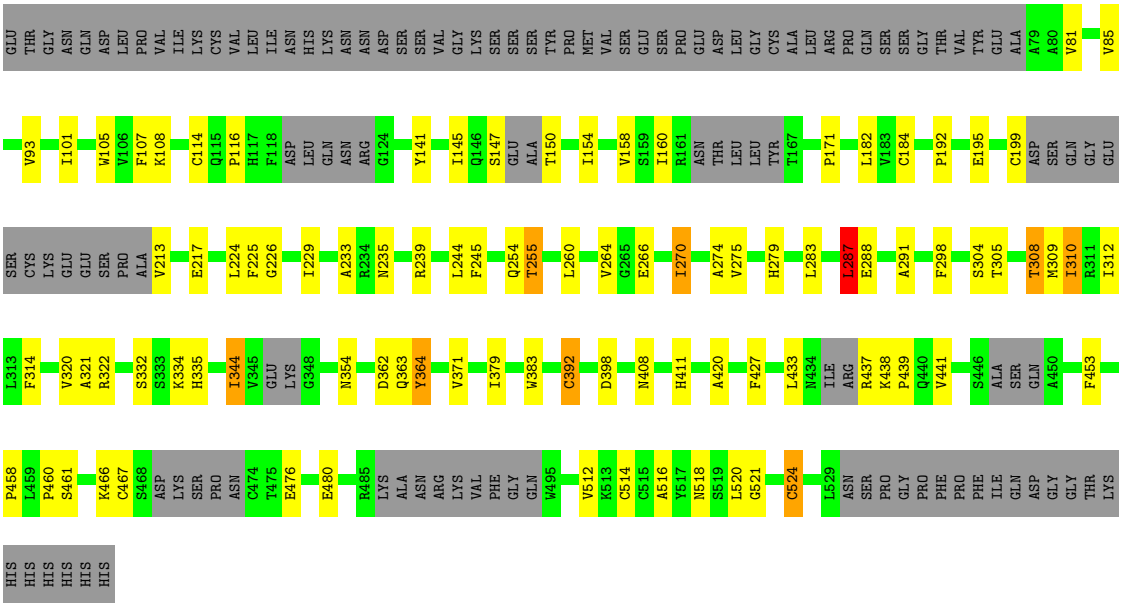
Chain D:



• Molecule 2: FL cytokine receptor

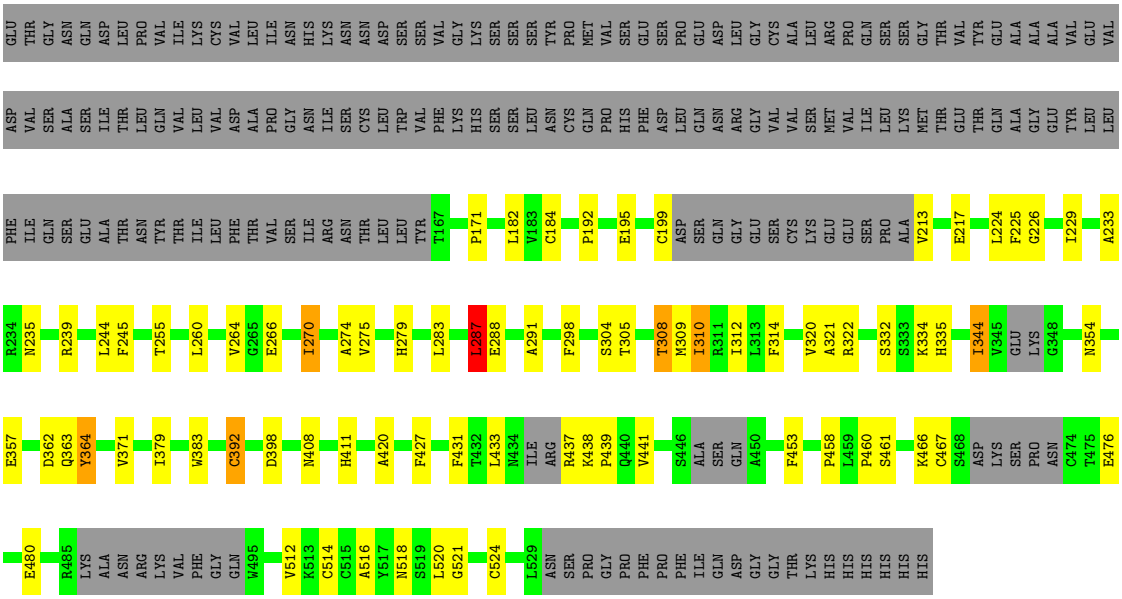
Chain E:





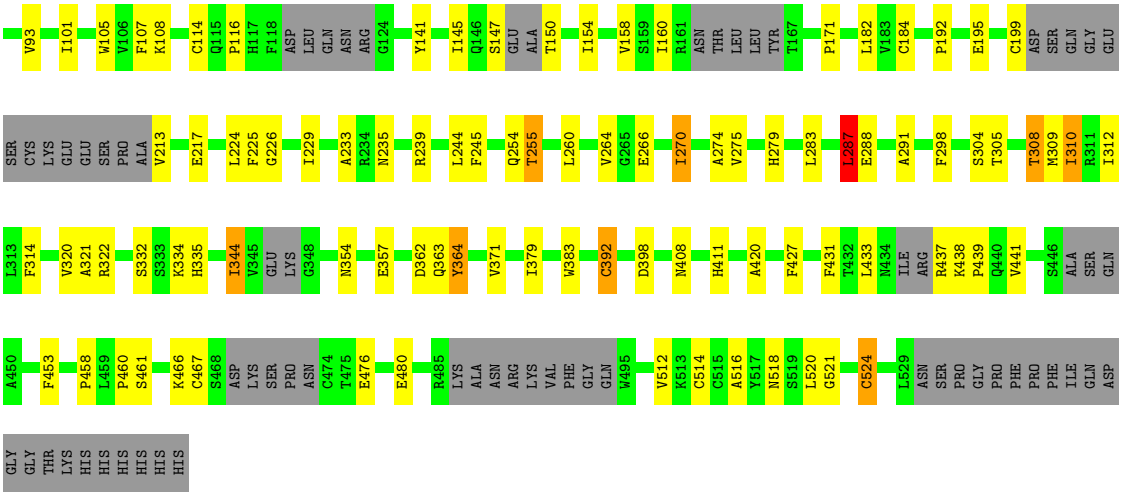
- Molecule 2: FL cytokine receptor

Chain F:



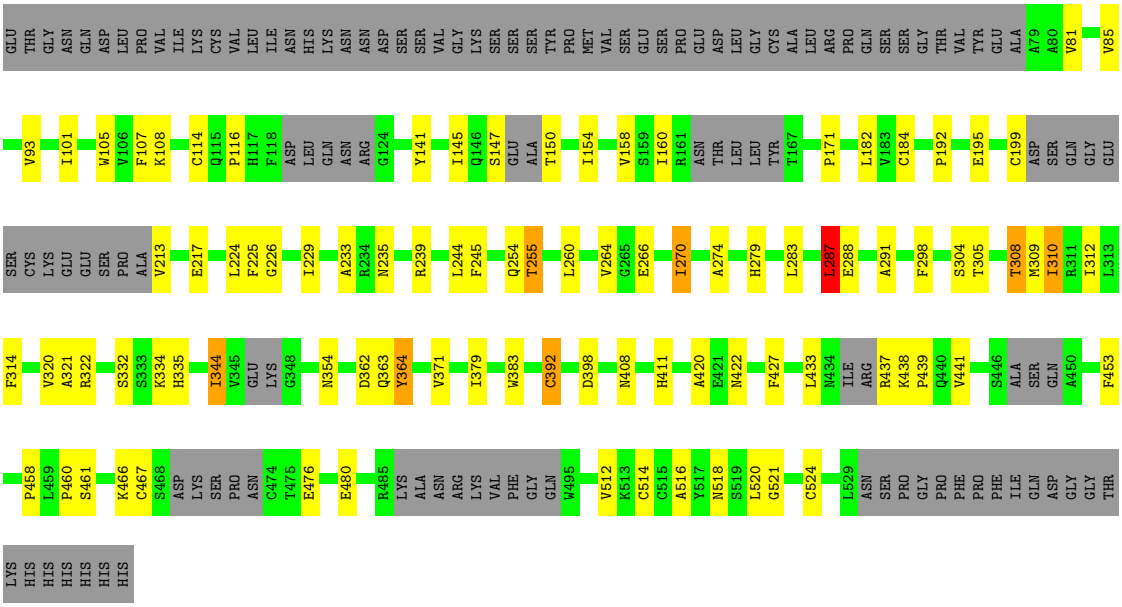
- Molecule 2: FL cytokine receptor

Chain G:



- Molecule 2: FL cytokine receptor

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.75Å 153.55Å 133.87Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	35.00 – 7.80 39.52 – 7.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.00-7.80) 97.9 (39.52-7.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 8.26Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.337 , 0.346 0.350 , 0.403	Depositor DCC
R_{free} test set	568 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	422.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 566.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.64	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å^2)	363.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 (i)

5.1 Standard geometry (i)

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	0.33	0/1053	0.53	0/1428
1	B	0.34	0/1053	0.53	0/1428
1	C	0.33	0/1053	0.53	0/1428
1	D	0.34	0/1053	0.53	0/1428
2	E	0.62	0/2506	0.80	0/3464
2	F	0.64	0/2061	0.83	0/2848
2	G	0.62	0/2506	0.80	0/3464
2	H	0.62	0/2506	0.80	0/3464
All	All	0.55	0/13791	0.74	0/18952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1033	0	1027	23	0
1	B	1033	0	1027	22	0
1	C	1033	0	1027	22	0
1	D	1033	0	1027	21	0
2	E	2463	0	1750	57	0
2	F	2021	0	1430	52	0
2	G	2463	0	1750	58	0
2	H	2463	0	1750	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13542	0	10788	300	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 12.

All (300) 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:H:287:LEU:HD23	2:H:288:GLU:H	1.38	0.88
2:G:287:LEU:HD23	2:G:288:GLU:H	1.38	0.88
2:E:287:LEU:HD23	2:E:288:GLU:H	1.38	0.86
2:F:287:LEU:HD23	2:F:288:GLU:H	1.38	0.86
2:F:520:LEU:HD12	2:F:521:GLY:N	1.96	0.81
2:H:438:LYS:HA	2:H:520:LEU:CD1	2.11	0.81
2:G:438:LYS:HA	2:G:520:LEU:CD1	2.11	0.81
2:E:438:LYS:HA	2:E:520:LEU:CD1	2.11	0.81
2:E:520:LEU:HD12	2:E:521:GLY:N	1.96	0.81
2:F:438:LYS:HA	2:F:520:LEU:CD1	2.11	0.80
1:B:106:GLN:HA	1:B:106:GLN:HE21	1.46	0.80
2:G:520:LEU:HD12	2:G:521:GLY:N	1.96	0.80
2:H:520:LEU:HD12	2:H:521:GLY:N	1.96	0.80
1:C:106:GLN:HE21	1:C:106:GLN:HA	1.47	0.79
2:E:514:CYS:O	2:E:524:CYS:SG	2.41	0.79
2:G:514:CYS:O	2:G:524:CYS:SG	2.41	0.79
1:D:106:GLN:HE21	1:D:106:GLN:HA	1.46	0.78
2:F:514:CYS:O	2:F:524:CYS:SG	2.41	0.78
2:H:514:CYS:O	2:H:524:CYS:SG	2.41	0.78
1:A:106:GLN:HA	1:A:106:GLN:HE21	1.47	0.77
1:A:88:GLN:HE21	1:A:88:GLN:HA	1.50	0.76
1:B:88:GLN:HE21	1:B:88:GLN:HA	1.50	0.75
1:C:88:GLN:HE21	1:C:88:GLN:HA	1.50	0.74
1:D:88:GLN:HA	1:D:88:GLN:HE21	1.50	0.74
2:E:520:LEU:HD12	2:E:521:GLY:H	1.53	0.73
2:F:520:LEU:HD12	2:F:521:GLY:H	1.53	0.73
2:E:304:SER:HB2	2:E:310:ILE:HD11	1.71	0.73
2:F:304:SER:HB2	2:F:310:ILE:HD11	1.71	0.72
2:G:322:ARG:HA	2:G:344:ILE:HG21	1.71	0.72
2:F:322:ARG:HA	2:F:344:ILE:HG21	1.71	0.71
2:G:304:SER:HB2	2:G:310:ILE:HD11	1.71	0.71
2:E:322:ARG:HA	2:E:344:ILE:HG21	1.71	0.71
2:H:304:SER:HB2	2:H:310:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:520:LEU:HD12	2:G:521:GLY:H	1.53	0.70
2:H:322:ARG:HA	2:H:344:ILE:HG21	1.71	0.70
2:H:520:LEU:HD12	2:H:521:GLY:H	1.53	0.70
2:E:147:SER:HG	2:E:150:THR:N	1.89	0.70
2:F:466:LYS:CB	2:F:512:VAL:HG12	2.23	0.69
2:H:466:LYS:CB	2:H:512:VAL:HG12	2.24	0.68
2:E:466:LYS:CB	2:E:512:VAL:HG12	2.24	0.68
2:G:466:LYS:CB	2:G:512:VAL:HG12	2.23	0.68
2:G:147:SER:HG	2:G:150:THR:N	1.91	0.68
2:H:147:SER:HG	2:H:150:THR:N	1.93	0.67
2:E:437:ARG:O	2:E:520:LEU:HD11	1.96	0.66
2:H:379:ILE:HD13	2:H:420:ALA:HB1	1.78	0.65
2:F:437:ARG:O	2:F:520:LEU:HD11	1.97	0.65
2:G:379:ILE:HD13	2:G:420:ALA:HB1	1.78	0.65
2:E:379:ILE:HD13	2:E:420:ALA:HB1	1.78	0.64
2:H:437:ARG:O	2:H:520:LEU:HD11	1.96	0.64
2:G:437:ARG:O	2:G:520:LEU:HD11	1.96	0.64
2:F:379:ILE:HD13	2:F:420:ALA:HB1	1.78	0.64
1:C:20:ARG:HD2	1:C:21:GLU:HG3	1.80	0.64
1:A:20:ARG:HD2	1:A:21:GLU:HG3	1.80	0.64
2:G:438:LYS:HA	2:G:520:LEU:HD11	1.80	0.63
1:D:20:ARG:HD2	1:D:21:GLU:HG3	1.79	0.63
1:B:20:ARG:HD2	1:B:21:GLU:HG3	1.79	0.62
2:F:438:LYS:HA	2:F:520:LEU:HD13	1.81	0.62
2:G:439:PRO:CG	2:G:518:ASN:HB2	2.29	0.62
2:F:438:LYS:HA	2:F:520:LEU:HD11	1.81	0.62
2:F:439:PRO:CG	2:F:518:ASN:HB2	2.30	0.62
2:E:438:LYS:HA	2:E:520:LEU:HD11	1.81	0.62
2:H:438:LYS:HA	2:H:520:LEU:HD13	1.81	0.62
2:E:439:PRO:CG	2:E:518:ASN:HB2	2.30	0.62
2:H:439:PRO:CG	2:H:518:ASN:HB2	2.30	0.61
1:C:122:GLN:HB2	1:C:124:PHE:CZ	2.36	0.61
2:E:438:LYS:HA	2:E:520:LEU:HD13	1.81	0.61
1:A:122:GLN:HB2	1:A:124:PHE:CZ	2.36	0.61
2:H:438:LYS:HA	2:H:520:LEU:HD11	1.80	0.61
2:G:182:LEU:HB2	2:G:224:LEU:HD21	1.84	0.60
2:G:438:LYS:HA	2:G:520:LEU:HD13	1.81	0.60
1:B:122:GLN:HB2	1:B:124:PHE:CZ	2.37	0.60
1:D:122:GLN:HB2	1:D:124:PHE:CZ	2.37	0.60
2:F:182:LEU:HB2	2:F:224:LEU:HD21	1.84	0.60
2:H:182:LEU:HB2	2:H:224:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:LEU:HB2	2:E:224:LEU:HD21	1.84	0.59
2:E:518:ASN:OD1	2:E:520:LEU:HG	2.02	0.59
2:H:518:ASN:OD1	2:H:520:LEU:HG	2.02	0.59
2:F:441:VAL:HG23	2:F:453:PHE:O	2.03	0.59
2:F:518:ASN:OD1	2:F:520:LEU:HG	2.02	0.59
2:G:441:VAL:HG23	2:G:453:PHE:O	2.03	0.59
2:F:171:PRO:HB3	2:F:184:CYS:SG	2.43	0.59
2:G:171:PRO:HB3	2:G:184:CYS:SG	2.43	0.59
2:H:171:PRO:HB3	2:H:184:CYS:SG	2.43	0.59
2:E:441:VAL:HG23	2:E:453:PHE:O	2.03	0.59
2:G:518:ASN:OD1	2:G:520:LEU:HG	2.02	0.58
1:C:119:ILE:HG23	1:C:120:THR:HG23	1.85	0.58
1:D:17:VAL:O	1:D:20:ARG:HG3	2.03	0.58
2:E:171:PRO:HB3	2:E:184:CYS:SG	2.43	0.58
1:A:119:ILE:HG23	1:A:120:THR:HG23	1.85	0.58
2:E:332:SER:CB	2:E:335:HIS:HB2	2.34	0.58
2:H:332:SER:CB	2:H:335:HIS:HB2	2.34	0.58
2:H:441:VAL:HG23	2:H:453:PHE:O	2.03	0.58
2:E:441:VAL:O	2:E:441:VAL:HG13	2.04	0.58
2:G:320:VAL:HB	2:G:344:ILE:HD11	1.85	0.57
2:H:441:VAL:O	2:H:441:VAL:HG13	2.04	0.57
1:C:17:VAL:O	1:C:20:ARG:HG3	2.05	0.57
1:B:17:VAL:O	1:B:20:ARG:HG3	2.03	0.57
2:E:320:VAL:HB	2:E:344:ILE:HD11	1.85	0.57
2:F:320:VAL:HB	2:F:344:ILE:HD11	1.85	0.57
2:F:332:SER:CB	2:F:335:HIS:HB2	2.34	0.57
2:H:320:VAL:HB	2:H:344:ILE:HD11	1.85	0.57
2:F:441:VAL:HG13	2:F:441:VAL:O	2.04	0.57
2:G:332:SER:CB	2:G:335:HIS:HB2	2.34	0.57
1:D:119:ILE:HG23	1:D:120:THR:HG23	1.87	0.57
1:B:88:GLN:HA	1:B:88:GLN:NE2	2.19	0.57
2:E:466:LYS:CA	2:E:512:VAL:HG12	2.35	0.57
1:A:17:VAL:O	1:A:20:ARG:HG3	2.05	0.56
2:G:441:VAL:O	2:G:441:VAL:HG13	2.04	0.56
1:D:55:ARG:HH12	1:D:90:PRO:HD3	1.71	0.56
2:G:466:LYS:CA	2:G:512:VAL:HG12	2.35	0.56
2:H:466:LYS:CA	2:H:512:VAL:HG12	2.35	0.56
1:A:59:ARG:HH11	1:D:98:GLN:HE22	1.54	0.56
1:A:88:GLN:HA	1:A:88:GLN:NE2	2.20	0.56
2:F:466:LYS:CA	2:F:512:VAL:HG12	2.35	0.56
1:B:55:ARG:HH12	1:B:90:PRO:HD3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:245:PHE:HD2	2:E:270:ILE:HG23	1.71	0.55
2:G:245:PHE:HD2	2:G:270:ILE:HG23	1.72	0.55
1:B:98:GLN:HE22	1:C:59:ARG:HH11	1.54	0.55
1:B:119:ILE:HG23	1:B:120:THR:HG23	1.87	0.55
1:D:88:GLN:HA	1:D:88:GLN:NE2	2.19	0.55
1:A:55:ARG:HH12	1:A:90:PRO:HD3	1.72	0.55
2:G:287:LEU:CD2	2:G:288:GLU:H	2.16	0.54
2:H:287:LEU:CD2	2:H:288:GLU:H	2.16	0.54
2:F:458:PRO:O	2:F:460:PRO:HD3	2.07	0.54
2:H:199:CYS:HA	2:H:213:VAL:HA	1.90	0.54
2:E:458:PRO:O	2:E:460:PRO:HD3	2.07	0.54
2:H:245:PHE:HD2	2:H:270:ILE:HG23	1.71	0.54
1:C:55:ARG:HH12	1:C:90:PRO:HD3	1.72	0.54
2:F:245:PHE:HD2	2:F:270:ILE:HG23	1.71	0.54
2:E:437:ARG:O	2:E:520:LEU:HD21	2.08	0.54
2:G:437:ARG:O	2:G:520:LEU:HD21	2.08	0.53
2:F:287:LEU:CD2	2:F:288:GLU:H	2.16	0.53
2:F:437:ARG:O	2:F:520:LEU:HD21	2.08	0.53
2:E:199:CYS:HA	2:E:213:VAL:HA	1.90	0.53
2:E:101:ILE:HG12	2:E:147:SER:HA	1.91	0.53
1:D:117:PRO:HG2	1:D:118:TRP:CD1	2.44	0.53
2:G:458:PRO:O	2:G:460:PRO:HD3	2.08	0.53
2:H:458:PRO:O	2:H:460:PRO:HD3	2.08	0.53
2:F:199:CYS:HA	2:F:213:VAL:HA	1.90	0.53
1:C:117:PRO:HG2	1:C:118:TRP:CD1	2.44	0.53
2:G:199:CYS:HA	2:G:213:VAL:HA	1.90	0.53
1:A:117:PRO:HG2	1:A:118:TRP:CD1	2.44	0.53
1:C:88:GLN:HA	1:C:88:GLN:NE2	2.20	0.53
2:G:466:LYS:HA	2:G:512:VAL:HG12	1.91	0.52
2:H:437:ARG:O	2:H:520:LEU:HD21	2.08	0.52
2:F:466:LYS:HA	2:F:512:VAL:HG12	1.91	0.52
2:H:101:ILE:HG12	2:H:147:SER:HA	1.91	0.52
2:H:466:LYS:HA	2:H:512:VAL:HG12	1.91	0.52
1:A:106:GLN:HA	1:A:106:GLN:NE2	2.22	0.52
2:H:439:PRO:HD3	2:H:520:LEU:HD11	1.92	0.52
2:E:439:PRO:HD3	2:E:520:LEU:HD11	1.92	0.52
2:E:466:LYS:HA	2:E:512:VAL:HG12	1.91	0.52
1:B:117:PRO:HG2	1:B:118:TRP:CD1	2.44	0.52
2:F:439:PRO:HG3	2:F:518:ASN:HB2	1.92	0.52
1:B:98:GLN:HE22	1:C:59:ARG:HD3	1.75	0.52
2:G:101:ILE:HG12	2:G:147:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:437:ARG:N	2:G:520:LEU:HD21	2.25	0.52
2:H:437:ARG:N	2:H:520:LEU:HD21	2.25	0.52
1:D:84:LYS:HE3	2:G:279:HIS:CE1	2.46	0.51
2:E:81:VAL:HB	2:E:158:VAL:HA	1.93	0.51
2:F:439:PRO:HD3	2:F:520:LEU:HD11	1.92	0.51
1:D:12:SER:O	1:D:15:PHE:HD2	1.94	0.51
2:E:298:PHE:HB3	2:E:314:PHE:CE1	2.46	0.51
2:G:225:PHE:HA	2:G:312:ILE:HD11	1.92	0.51
1:B:84:LYS:HE3	2:F:279:HIS:CE1	2.46	0.51
2:E:437:ARG:N	2:E:520:LEU:HD21	2.25	0.51
2:G:439:PRO:HD3	2:G:520:LEU:HD11	1.92	0.51
1:B:12:SER:O	1:B:15:PHE:HD2	1.93	0.51
2:E:439:PRO:HG3	2:E:518:ASN:HB2	1.92	0.51
2:F:298:PHE:HB3	2:F:314:PHE:CE1	2.46	0.51
2:F:437:ARG:N	2:F:520:LEU:HD21	2.25	0.51
2:G:439:PRO:HG3	2:G:518:ASN:HB2	1.92	0.51
2:H:245:PHE:CD2	2:H:270:ILE:HG23	2.46	0.51
2:H:439:PRO:HG3	2:H:518:ASN:HB2	1.92	0.51
2:E:225:PHE:HA	2:E:312:ILE:HD11	1.92	0.51
2:E:287:LEU:CD2	2:E:288:GLU:H	2.16	0.50
2:G:298:PHE:HB3	2:G:314:PHE:CE1	2.46	0.50
2:H:458:PRO:N	2:H:518:ASN:HD21	2.09	0.50
1:B:47:LEU:O	1:B:51:VAL:HG23	2.12	0.50
2:G:81:VAL:HB	2:G:158:VAL:HA	1.92	0.50
2:E:458:PRO:N	2:E:518:ASN:HD21	2.09	0.50
2:G:245:PHE:CD2	2:G:270:ILE:HG23	2.46	0.50
2:F:458:PRO:N	2:F:518:ASN:HD21	2.10	0.50
2:H:81:VAL:HB	2:H:158:VAL:HA	1.93	0.50
2:H:298:PHE:HB3	2:H:314:PHE:CE1	2.46	0.50
2:E:245:PHE:CD2	2:E:270:ILE:HG23	2.46	0.50
2:H:225:PHE:HA	2:H:312:ILE:HD11	1.92	0.50
1:C:47:LEU:O	1:C:51:VAL:HG23	2.12	0.50
1:C:84:LYS:HE3	2:H:279:HIS:CE1	2.47	0.50
1:D:47:LEU:O	1:D:51:VAL:HG23	2.11	0.50
2:F:245:PHE:CD2	2:F:270:ILE:HG23	2.46	0.50
1:A:84:LYS:HE3	2:E:279:HIS:CE1	2.47	0.49
2:G:458:PRO:N	2:G:518:ASN:HD21	2.10	0.49
2:F:225:PHE:HA	2:F:312:ILE:HD11	1.92	0.49
1:A:47:LEU:O	1:A:51:VAL:HG23	2.12	0.49
1:B:106:GLN:HA	1:B:106:GLN:NE2	2.21	0.49
2:F:264:VAL:HG13	2:F:321:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:VAL:HG13	2:E:321:ALA:HA	1.95	0.48
2:E:105:TRP:HD1	2:E:114:CYS:HB3	1.79	0.48
2:H:264:VAL:HG13	2:H:321:ALA:HA	1.95	0.48
1:D:106:GLN:HA	1:D:106:GLN:NE2	2.21	0.48
1:C:106:GLN:HA	1:C:106:GLN:NE2	2.23	0.48
2:H:105:TRP:HD1	2:H:114:CYS:HB3	1.79	0.48
1:D:50:LEU:HG	1:D:111:GLN:HE21	1.79	0.47
2:G:264:VAL:HG13	2:G:321:ALA:HA	1.95	0.47
1:B:50:LEU:HG	1:B:111:GLN:HE21	1.79	0.47
2:G:105:TRP:HD1	2:G:114:CYS:HB3	1.79	0.47
2:F:437:ARG:C	2:F:520:LEU:HD21	2.35	0.47
1:C:50:LEU:HG	1:C:111:GLN:HE21	1.80	0.47
2:E:437:ARG:C	2:E:520:LEU:HD21	2.35	0.47
1:A:12:SER:O	1:A:15:PHE:HD2	1.98	0.46
2:F:266:GLU:O	2:F:320:VAL:HG22	2.15	0.46
2:H:266:GLU:O	2:H:320:VAL:HG22	2.15	0.46
2:E:467:CYS:CB	2:E:476:GLU:CB	2.94	0.46
2:G:437:ARG:C	2:G:520:LEU:HD21	2.35	0.46
2:H:467:CYS:CB	2:H:476:GLU:CB	2.94	0.46
2:H:437:ARG:C	2:H:520:LEU:HD21	2.35	0.46
1:C:12:SER:O	1:C:15:PHE:HD2	1.99	0.46
2:F:467:CYS:CB	2:F:476:GLU:CB	2.94	0.46
1:A:50:LEU:HG	1:A:111:GLN:HE21	1.80	0.46
2:E:192:PRO:HB3	2:E:235:ASN:HB3	1.98	0.46
1:A:103:ARG:HA	1:A:103:ARG:HD2	1.73	0.45
1:A:18:LYS:HD2	1:A:18:LYS:N	2.31	0.45
2:G:192:PRO:HB3	2:G:235:ASN:HB3	1.98	0.45
1:C:18:LYS:HD2	1:C:18:LYS:N	2.31	0.45
2:H:192:PRO:HB3	2:H:235:ASN:HB3	1.98	0.45
1:A:37:ASN:OD1	1:A:94:LEU:HD12	2.17	0.45
2:F:461:SER:O	2:F:516:ALA:HA	2.17	0.45
2:G:467:CYS:CB	2:G:476:GLU:CB	2.94	0.45
2:H:107:PHE:HA	2:H:141:TYR:HD2	1.81	0.45
2:E:266:GLU:O	2:E:320:VAL:HG22	2.15	0.45
2:E:233:ALA:O	2:E:239:ARG:HA	2.17	0.45
1:C:10:PRO:HB3	2:H:279:HIS:CE1	2.53	0.44
2:G:107:PHE:HA	2:G:141:TYR:HD2	1.81	0.44
2:G:461:SER:O	2:G:516:ALA:HA	2.17	0.44
1:A:10:PRO:HB3	2:E:279:HIS:CE1	2.53	0.44
2:G:233:ALA:O	2:G:239:ARG:HA	2.17	0.44
2:E:107:PHE:HA	2:E:141:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:192:PRO:HB3	2:F:235:ASN:HB3	1.98	0.44
2:F:274:ALA:HB3	2:F:283:LEU:HD11	1.99	0.44
2:G:266:GLU:O	2:G:320:VAL:HG22	2.16	0.44
1:D:37:ASN:OD1	1:D:94:LEU:HD12	2.18	0.44
2:E:461:SER:O	2:E:516:ALA:HA	2.17	0.44
2:H:233:ALA:O	2:H:239:ARG:HA	2.17	0.44
1:B:37:ASN:OD1	1:B:94:LEU:HD12	2.18	0.44
2:G:274:ALA:HB3	2:G:283:LEU:HD11	1.99	0.44
2:H:461:SER:O	2:H:516:ALA:HA	2.17	0.44
2:F:233:ALA:O	2:F:239:ARG:HA	2.17	0.43
1:B:18:LYS:N	1:B:18:LYS:HD2	2.33	0.43
1:D:18:LYS:N	1:D:18:LYS:HD2	2.33	0.43
1:C:37:ASN:OD1	1:C:94:LEU:HD12	2.17	0.43
2:F:195:GLU:HA	2:F:217:GLU:HA	2.01	0.43
2:G:195:GLU:HA	2:G:217:GLU:HA	2.01	0.43
2:H:274:ALA:HB3	2:H:283:LEU:HD11	1.99	0.43
2:E:274:ALA:HB3	2:E:283:LEU:HD11	1.99	0.43
1:B:10:PRO:HB3	2:F:279:HIS:CE1	2.54	0.43
2:E:354:ASN:HB3	2:E:427:PHE:CE1	2.54	0.43
1:C:103:ARG:HD2	1:C:103:ARG:HA	1.73	0.43
1:A:24:ASP:O	1:B:67:LYS:HB2	2.19	0.43
1:D:10:PRO:HB3	2:G:279:HIS:CE1	2.54	0.43
2:E:195:GLU:HA	2:E:217:GLU:HA	2.01	0.42
2:H:362:ASP:O	2:H:364:TYR:N	2.53	0.42
2:F:354:ASN:HB3	2:F:427:PHE:CE1	2.54	0.42
2:G:354:ASN:HB3	2:G:427:PHE:CE1	2.54	0.42
2:H:195:GLU:HA	2:H:217:GLU:HA	2.01	0.42
1:D:103:ARG:HA	1:D:103:ARG:HD2	1.72	0.42
2:G:362:ASP:O	2:G:364:TYR:N	2.53	0.42
2:H:354:ASN:HB3	2:H:427:PHE:CE1	2.54	0.42
2:G:304:SER:HB3	2:G:308:THR:HB	2.02	0.42
2:H:304:SER:HB3	2:H:308:THR:HB	2.02	0.42
2:H:467:CYS:CB	2:H:476:GLU:H	2.33	0.42
1:B:48:TRP:CD1	1:B:130:LEU:HG	2.55	0.42
2:E:304:SER:HB3	2:E:308:THR:HB	2.02	0.42
1:A:88:GLN:HE21	1:A:89:PRO:HD2	1.85	0.41
1:C:48:TRP:CD1	1:C:130:LEU:HG	2.55	0.41
2:E:467:CYS:CB	2:E:476:GLU:H	2.33	0.41
1:B:88:GLN:HE21	1:B:89:PRO:HD2	1.85	0.41
1:C:88:GLN:HE21	1:C:89:PRO:HD2	1.85	0.41
2:E:362:ASP:O	2:E:364:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:275:VAL:HG22	2:E:310:ILE:HG23	2.02	0.41
1:D:48:TRP:CD1	1:D:130:LEU:HG	2.55	0.41
2:G:467:CYS:CB	2:G:476:GLU:H	2.33	0.41
1:A:106:GLN:HE21	1:A:106:GLN:CA	2.23	0.41
1:D:88:GLN:HE21	1:D:89:PRO:HD2	1.86	0.41
2:F:304:SER:HB3	2:F:308:THR:HB	2.02	0.41
2:F:362:ASP:O	2:F:364:TYR:N	2.53	0.41
2:F:467:CYS:CB	2:F:476:GLU:H	2.33	0.41
2:H:383:TRP:CD1	2:H:392:CYS:HB3	2.56	0.41
2:F:275:VAL:HG22	2:F:310:ILE:HG23	2.02	0.40
2:F:383:TRP:CD1	2:F:392:CYS:HB3	2.56	0.40
2:H:254:GLN:O	2:H:255:THR:C	2.60	0.40
1:A:48:TRP:CD1	1:A:130:LEU:HG	2.55	0.40
2:E:254:GLN:O	2:E:255:THR:C	2.59	0.40
2:G:383:TRP:CD1	2:G:392:CYS:HB3	2.56	0.40
2:H:379:ILE:HG22	2:H:422:ASN:HB3	2.04	0.40
2:G:254:GLN:O	2:G:255:THR:C	2.60	0.40
2:G:275:VAL:HG22	2:G:310:ILE:HG23	2.02	0.40
2:E:383:TRP:CD1	2:E:392:CYS:HB3	2.56	0.40
2:F:357:GLU:O	2:F:431:PHE:HA	2.22	0.40
2:G:357:GLU:O	2:G:431:PHE:HA	2.22	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	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	19 60
1	B	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	19 60
1	C	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	19 60
1	D	128/138 (93%)	120 (94%)	7 (6%)	1 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	3	23
2	F	315/527 (60%)	273 (87%)	30 (10%)	12 (4%)	3	24
2	G	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	3	23
2	H	385/527 (73%)	333 (86%)	37 (10%)	15 (4%)	3	23
All	All	1982/2660 (74%)	1752 (88%)	169 (8%)	61 (3%)	4	27

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	85	VAL
2	E	255	THR
2	E	305	THR
2	E	334	LYS
2	E	363	GLN
2	F	255	THR
2	F	305	THR
2	F	334	LYS
2	F	363	GLN
2	G	85	VAL
2	G	255	THR
2	G	305	THR
2	G	334	LYS
2	G	363	GLN
2	H	85	VAL
2	H	255	THR
2	H	305	THR
2	H	334	LYS
2	H	363	GLN
2	E	291	ALA
2	F	291	ALA
2	G	291	ALA
2	H	291	ALA
2	E	108	LYS
2	E	226	GLY
2	E	364	TYR
2	F	226	GLY
2	F	364	TYR
2	G	108	LYS
2	G	226	GLY
2	G	364	TYR
2	H	108	LYS

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Mol	Chain	Res	Type
2	H	364	TYR
1	A	42	GLU
1	C	42	GLU
2	E	398	ASP
2	E	408	ASN
2	E	480	GLU
2	F	398	ASP
2	F	408	ASN
2	F	480	GLU
2	G	398	ASP
2	G	408	ASN
2	G	480	GLU
2	H	226	GLY
2	H	398	ASP
2	H	408	ASN
2	H	480	GLU
1	B	42	GLU
1	D	42	GLU
2	E	411	HIS
2	F	411	HIS
2	G	411	HIS
2	H	411	HIS
2	E	116	PRO
2	E	287	LEU
2	F	287	LEU
2	G	116	PRO
2	G	287	LEU
2	H	116	PRO
2	H	287	LEU

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	115/127 (91%)	111 (96%)	4 (4%)	36 59
1	B	115/127 (91%)	111 (96%)	4 (4%)	36 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	115/127 (91%)	111 (96%)	4 (4%)	36	59
1	D	115/127 (91%)	111 (96%)	4 (4%)	36	59
2	E	139/473 (29%)	122 (88%)	17 (12%)	5	20
2	F	117/473 (25%)	105 (90%)	12 (10%)	7	25
2	G	139/473 (29%)	122 (88%)	17 (12%)	5	20
2	H	139/473 (29%)	123 (88%)	16 (12%)	5	21
All	All	994/2400 (41%)	916 (92%)	78 (8%)	12	36

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	20	ARG
1	A	88	GLN
1	A	106	GLN
1	B	18	LYS
1	B	20	ARG
1	B	88	GLN
1	B	106	GLN
1	C	18	LYS
1	C	20	ARG
1	C	88	GLN
1	C	106	GLN
1	D	18	LYS
1	D	20	ARG
1	D	88	GLN
1	D	106	GLN
2	E	93	VAL
2	E	145	ILE
2	E	154	ILE
2	E	160	ILE
2	E	229	ILE
2	E	244	LEU
2	E	260	LEU
2	E	270	ILE
2	E	287	LEU
2	E	308	THR
2	E	309	MET
2	E	310	ILE
2	E	344	ILE

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Mol	Chain	Res	Type
2	E	371	VAL
2	E	392	CYS
2	E	433	LEU
2	E	524	CYS
2	F	229	ILE
2	F	244	LEU
2	F	260	LEU
2	F	270	ILE
2	F	287	LEU
2	F	308	THR
2	F	309	MET
2	F	310	ILE
2	F	344	ILE
2	F	371	VAL
2	F	392	CYS
2	F	433	LEU
2	G	93	VAL
2	G	145	ILE
2	G	154	ILE
2	G	160	ILE
2	G	229	ILE
2	G	244	LEU
2	G	260	LEU
2	G	270	ILE
2	G	287	LEU
2	G	308	THR
2	G	309	MET
2	G	310	ILE
2	G	344	ILE
2	G	371	VAL
2	G	392	CYS
2	G	433	LEU
2	G	524	CYS
2	H	93	VAL
2	H	145	ILE
2	H	154	ILE
2	H	160	ILE
2	H	229	ILE
2	H	244	LEU
2	H	260	LEU
2	H	270	ILE
2	H	287	LEU

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Mol	Chain	Res	Type
2	H	308	THR
2	H	309	MET
2	H	310	ILE
2	H	344	ILE
2	H	371	VAL
2	H	392	CYS
2	H	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	80	HIS
1	A	88	GLN
1	A	106	GLN
1	A	111	GLN
1	A	122	GLN
1	B	28	GLN
1	B	80	HIS
1	B	88	GLN
1	B	98	GLN
1	B	106	GLN
1	B	111	GLN
1	B	122	GLN
1	C	28	GLN
1	C	80	HIS
1	C	88	GLN
1	C	106	GLN
1	C	111	GLN
1	C	122	GLN
1	D	28	GLN
1	D	80	HIS
1	D	88	GLN
1	D	98	GLN
1	D	106	GLN
1	D	111	GLN
1	D	122	GLN
2	E	279	HIS
2	F	279	HIS
2	G	279	HIS
2	H	279	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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