



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:03 AM GMT

PDB ID : 2O7U  
Title : Crystal structure of K206E/K296E mutant of the N-terminal half molecule of human transferrin  
Authors : Baker, H.M.; Nurizzo, D.; Mason, A.B.; Baker, E.N.  
Deposited on : 2006-12-11  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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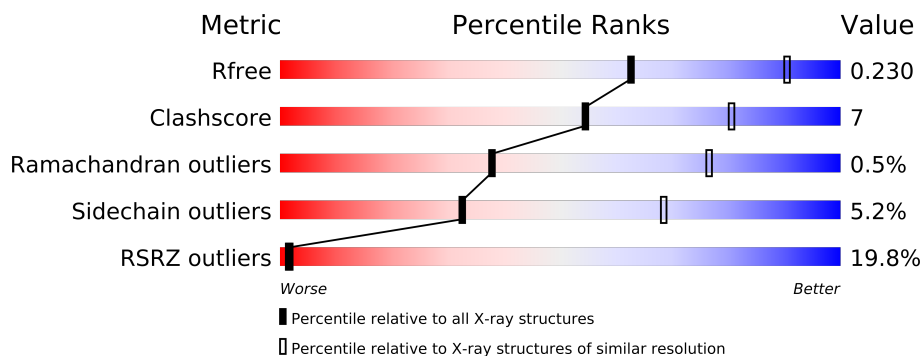
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	
1	E	337	
1	F	337	
1	G	337	
1	H	337	
1	I	337	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23067 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	A	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	C	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	D	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	E	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	F	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	G	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	H	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			
1	I	329	Total	C	N	O	S	0	0	0
			2550	1610	435	484	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	GLU	LYS	ENGINEERED	UNP P02787
B	296	GLU	LYS	ENGINEERED	UNP P02787
A	206	GLU	LYS	ENGINEERED	UNP P02787
A	296	GLU	LYS	ENGINEERED	UNP P02787
C	206	GLU	LYS	ENGINEERED	UNP P02787
C	296	GLU	LYS	ENGINEERED	UNP P02787
D	206	GLU	LYS	ENGINEERED	UNP P02787
D	296	GLU	LYS	ENGINEERED	UNP P02787
E	206	GLU	LYS	ENGINEERED	UNP P02787
E	296	GLU	LYS	ENGINEERED	UNP P02787
F	206	GLU	LYS	ENGINEERED	UNP P02787

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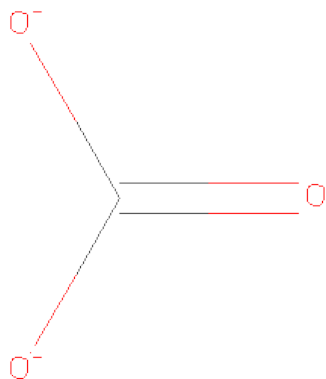
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Chain	Residue	Modelled	Actual	Comment	Reference
F	296	GLU	LYS	ENGINEERED	UNP P02787
G	206	GLU	LYS	ENGINEERED	UNP P02787
G	296	GLU	LYS	ENGINEERED	UNP P02787
H	206	GLU	LYS	ENGINEERED	UNP P02787
H	296	GLU	LYS	ENGINEERED	UNP P02787
I	206	GLU	LYS	ENGINEERED	UNP P02787
I	296	GLU	LYS	ENGINEERED	UNP P02787

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	10	Total	O	0	0
			10	10		
4	C	8	Total	O	0	0
			8	8		

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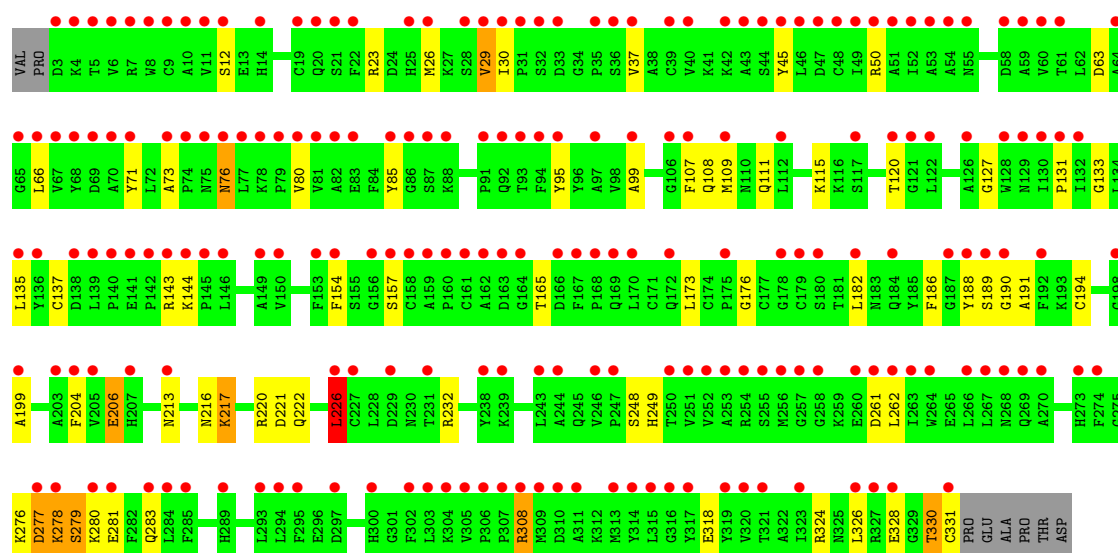
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	10	Total 10	O 10	0	0
4	E	10	Total 10	O 10	0	0
4	F	10	Total 10	O 10	0	0
4	G	2	Total 2	O 2	0	0
4	H	8	Total 8	O 8	0	0
4	I	5	Total 5	O 5	0	0

### 3 Residue-property plots

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.

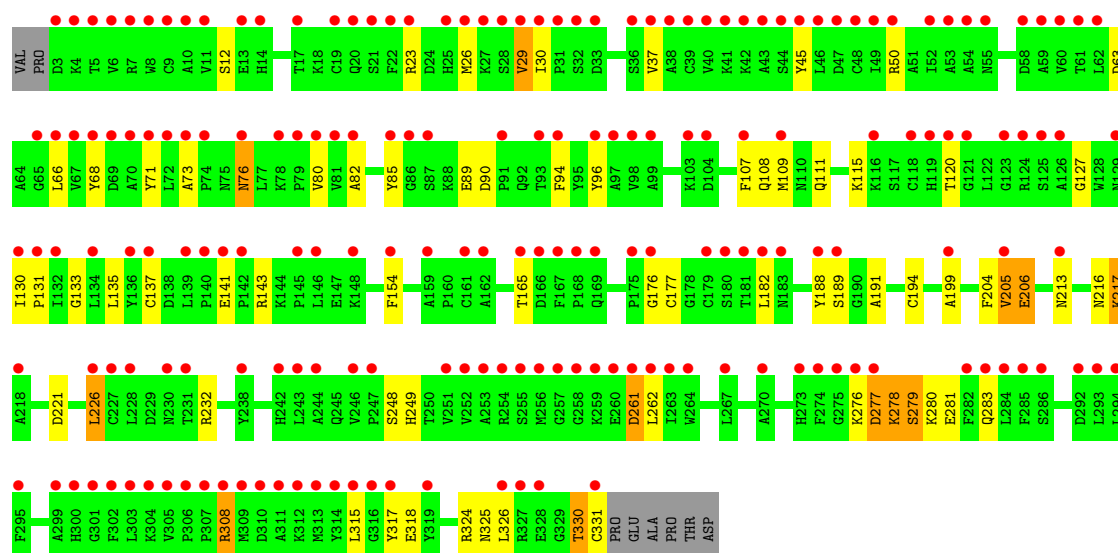
#### • Molecule 1: Serotransferrin

Chain B: 

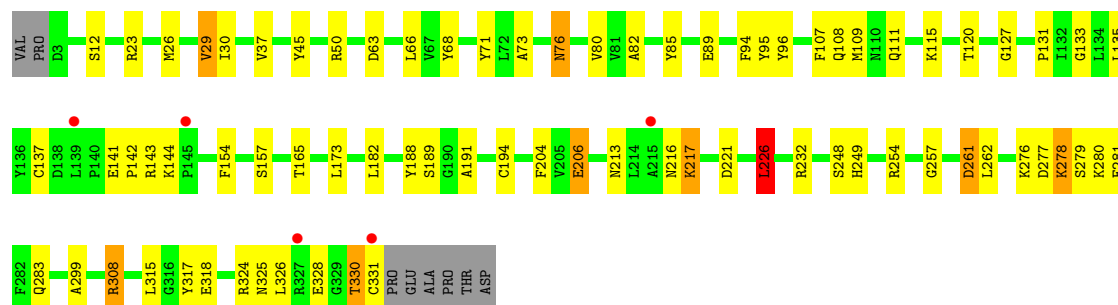


#### • Molecule 1: Serotransferrin

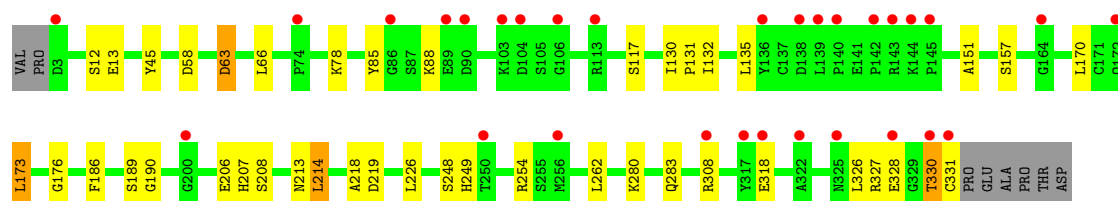
Chain A: 



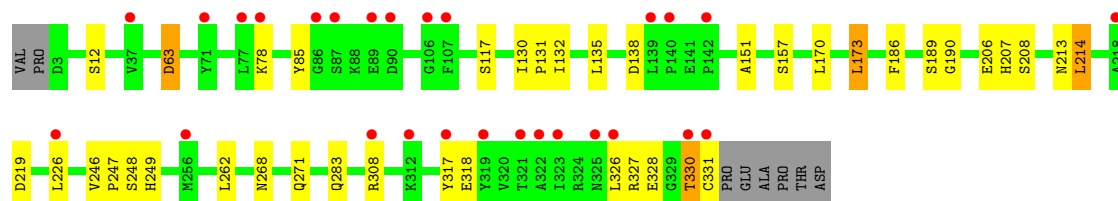
- Molecule 1: Serotransferrin

Chain C: 

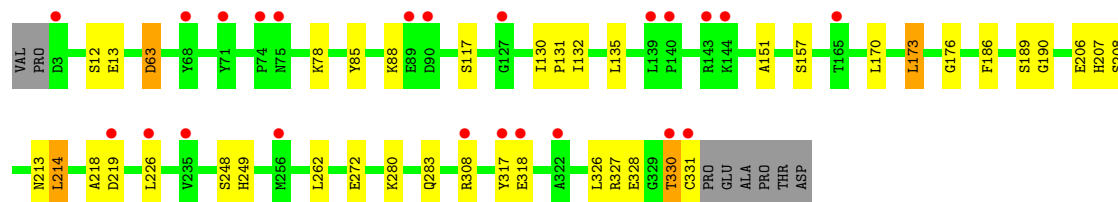
- Molecule 1: Serotransferrin

Chain D: 

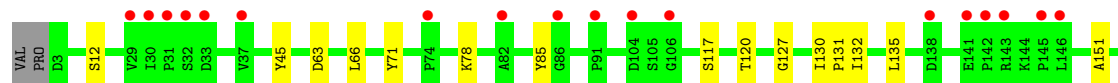
- Molecule 1: Serotransferrin

Chain E: 

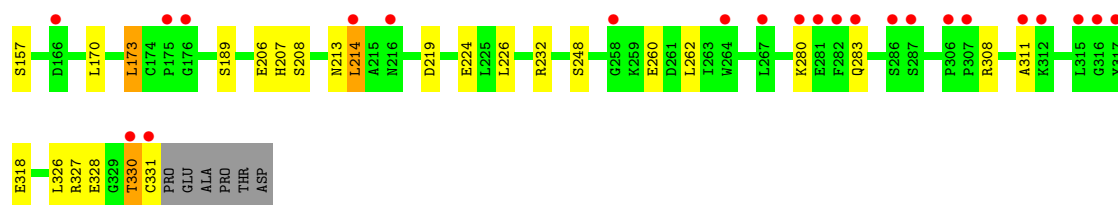
- Molecule 1: Serotransferrin

Chain F: 

- Molecule 1: Serotransferrin

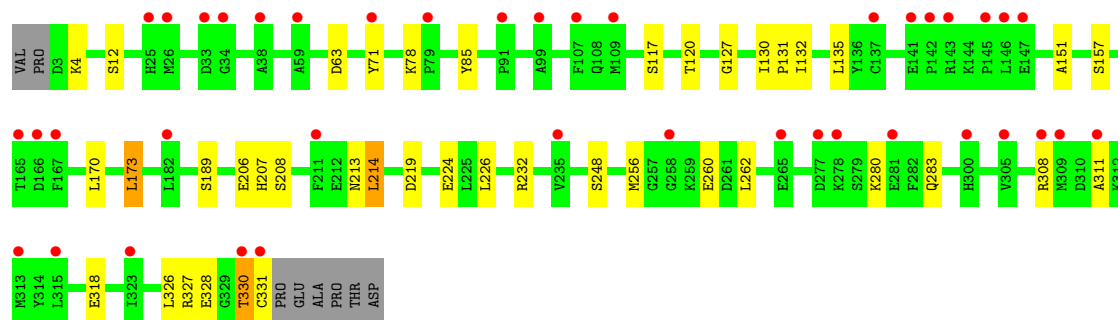
Chain G: 





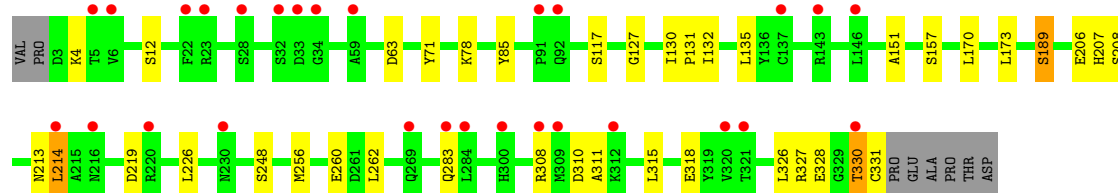
• Molecule 1: Serotransferrin

Chain H:



• Molecule 1: Serotransferrin

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.46Å 97.90Å 208.95Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	29.76 – 2.80 29.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.76-2.80) 97.2 (29.76-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, $R_{free}$	0.230 , 0.259 0.222 , 0.230	Depositor DCC
$R_{free}$ test set	4162 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 90.8	EDS
Estimated twinning fraction	0.036 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.036 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.440 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.439 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.032 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 82144 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	23067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, 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	0.61	1/2611 (0.0%)	0.74	2/3532 (0.1%)
1	B	0.61	0/2611	0.71	1/3532 (0.0%)
1	C	0.61	0/2611	0.71	1/3532 (0.0%)
1	D	0.55	0/2611	0.64	0/3532
1	E	0.55	0/2611	0.63	0/3532
1	F	0.55	0/2611	0.64	0/3532
1	G	0.51	0/2611	0.61	0/3532
1	H	0.51	0/2611	0.61	0/3532
1	I	0.49	0/2611	0.60	0/3532
All	All	0.56	1/23499 (0.0%)	0.66	4/31788 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	CYS	CB-SG	-5.45	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLU	CA-CB-CG	6.41	127.50	113.40
1	C	226	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	226	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	205	VAL	CB-CA-C	5.08	121.06	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2550	0	2453	62	1
1	B	2550	0	2453	47	0
1	C	2550	0	2453	68	0
1	D	2550	0	2453	29	0
1	E	2550	0	2453	26	0
1	F	2550	0	2453	30	1
1	G	2550	0	2453	23	0
1	H	2550	0	2453	36	0
1	I	2550	0	2453	34	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	1	0
4	A	9	0	0	0	0
4	B	10	0	0	0	0
4	C	8	0	0	0	0
4	D	10	0	0	1	0
4	E	10	0	0	0	0
4	F	10	0	0	1	0
4	G	2	0	0	0	0
4	H	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	5	0	0	0	0
All	All	23067	0	22077	305	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (305) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:218:ALA:CB	1:F:218:ALA:HB2	1.93	0.98
1:D:218:ALA:HB2	1:F:218:ALA:CB	1.95	0.96
1:D:218:ALA:HB2	1:F:218:ALA:HB1	1.49	0.92
1:D:218:ALA:HB1	1:F:218:ALA:HB2	1.51	0.92
1:A:82:ALA:HB3	1:I:256:MET:HE1	1.52	0.90
1:D:218:ALA:CB	1:F:218:ALA:CB	2.48	0.89
1:C:82:ALA:HB3	1:H:256:MET:HE1	1.58	0.85
1:A:108:GLN:HE22	1:A:232:ARG:HG3	1.41	0.83
1:A:82:ALA:HB3	1:I:256:MET:CE	2.10	0.81
1:B:108:GLN:HE22	1:B:232:ARG:HG3	1.48	0.79
1:C:108:GLN:HE22	1:C:232:ARG:HG3	1.48	0.78
1:C:82:ALA:HB3	1:H:256:MET:CE	2.14	0.76
1:A:109:MET:HE2	1:A:226:LEU:HB3	1.69	0.75
1:B:308:ARG:HG2	1:B:308:ARG:HH11	1.51	0.74
1:C:142:PRO:HD3	1:E:330:THR:HB	1.68	0.74
1:C:308:ARG:HG2	1:C:308:ARG:HH11	1.52	0.73
1:A:308:ARG:HH11	1:A:308:ARG:HG2	1.54	0.72
1:I:308:ARG:O	1:I:308:ARG:HG2	1.90	0.72
1:C:94:PHE:HZ	1:H:308:ARG:HB2	1.54	0.71
1:B:330:THR:HG22	1:B:331:CYS:H	1.56	0.71
1:C:94:PHE:CZ	1:H:308:ARG:HB2	2.26	0.71
1:B:109:MET:HE2	1:B:226:LEU:HB3	1.72	0.70
1:G:308:ARG:HG2	1:G:308:ARG:O	1.91	0.70
1:H:330:THR:HG22	1:H:331:CYS:H	1.57	0.70
1:A:94:PHE:HZ	1:I:308:ARG:HB2	1.57	0.70
1:H:308:ARG:HG2	1:H:308:ARG:O	1.91	0.70
1:I:330:THR:HG22	1:I:331:CYS:H	1.57	0.69
1:C:330:THR:HG22	1:C:331:CYS:H	1.58	0.69
1:A:107:PHE:HB3	1:A:115:LYS:HE3	1.75	0.69
1:A:330:THR:HG22	1:A:331:CYS:H	1.58	0.69
1:C:107:PHE:HB3	1:C:115:LYS:HE3	1.75	0.68
1:G:330:THR:HG22	1:G:331:CYS:H	1.58	0.68
1:B:107:PHE:HB3	1:B:115:LYS:HE3	1.76	0.68
1:A:94:PHE:CZ	1:I:308:ARG:HB2	2.29	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:214:LEU:HD11	1:F:219:ASP:HB2	1.75	0.67
1:C:63:ASP:HA	1:C:249:HIS:CD2	2.30	0.66
1:C:94:PHE:CZ	1:H:308:ARG:HG3	2.30	0.66
1:D:214:LEU:HD11	1:D:219:ASP:HB2	1.77	0.65
1:B:308:ARG:O	1:B:308:ARG:HG2	1.96	0.65
1:G:326:LEU:O	1:G:326:LEU:HG	1.96	0.65
1:F:308:ARG:O	1:F:308:ARG:HG2	1.97	0.65
1:H:326:LEU:HG	1:H:326:LEU:O	1.96	0.65
1:I:326:LEU:HG	1:I:326:LEU:O	1.96	0.65
1:E:214:LEU:HD11	1:E:219:ASP:HB2	1.78	0.64
1:E:308:ARG:O	1:E:308:ARG:HG2	1.96	0.64
1:H:214:LEU:HD11	1:H:219:ASP:HB2	1.79	0.64
1:C:109:MET:HE2	1:C:226:LEU:HB3	1.79	0.64
1:A:308:ARG:HG2	1:A:308:ARG:O	1.97	0.64
1:A:23:ARG:HA	1:A:37:VAL:CG1	2.29	0.63
1:B:63:ASP:HA	1:B:249:HIS:CD2	2.34	0.63
1:C:308:ARG:HG2	1:C:308:ARG:O	1.99	0.62
1:C:94:PHE:HZ	1:H:308:ARG:CG	2.12	0.62
1:A:96:TYR:OH	1:I:308:ARG:HD2	1.99	0.62
1:C:141:GLU:O	1:E:330:THR:CB	2.48	0.62
1:C:96:TYR:OH	1:H:308:ARG:HD2	2.00	0.62
1:D:326:LEU:HG	1:D:326:LEU:O	2.00	0.62
1:I:214:LEU:HD11	1:I:219:ASP:HB2	1.82	0.62
1:A:82:ALA:CB	1:I:256:MET:CE	2.76	0.62
1:C:94:PHE:HZ	1:H:308:ARG:CB	2.13	0.62
1:C:23:ARG:HA	1:C:37:VAL:CG1	2.30	0.62
1:F:151:ALA:HB2	1:F:170:LEU:HG	1.81	0.62
1:A:89:GLU:O	1:I:71:TYR:OH	2.18	0.61
1:E:130:ILE:HB	1:E:131:PRO:HD3	1.82	0.61
1:B:23:ARG:HA	1:B:37:VAL:CG1	2.30	0.61
1:F:130:ILE:HB	1:F:131:PRO:HD3	1.81	0.61
1:D:130:ILE:HB	1:D:131:PRO:HD3	1.82	0.61
1:C:82:ALA:CB	1:H:256:MET:CE	2.79	0.61
1:A:189:SER:HB2	1:A:213:ASN:OD1	2.01	0.61
1:A:94:PHE:CZ	1:I:308:ARG:HG3	2.35	0.61
1:E:151:ALA:HB2	1:E:170:LEU:HG	1.83	0.60
1:A:63:ASP:HA	1:A:249:HIS:CD2	2.36	0.60
1:F:326:LEU:HG	1:F:326:LEU:O	2.01	0.60
1:B:217:LYS:HE3	1:B:221:ASP:OD1	2.02	0.60
1:C:142:PRO:CD	1:E:330:THR:HB	2.31	0.59
1:C:189:SER:HB2	1:C:213:ASN:OD1	2.01	0.59
1:B:308:ARG:HH11	1:B:308:ARG:CG	2.16	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:LYS:HE3	1:A:221:ASP:OD1	2.02	0.59
1:E:326:LEU:O	1:E:326:LEU:HG	2.02	0.59
1:F:206:GLU:OE1	4:F:604:HOH:O	2.17	0.59
1:D:308:ARG:HG2	1:D:308:ARG:O	2.02	0.59
1:G:214:LEU:HD11	1:G:219:ASP:HB2	1.84	0.59
1:E:330:THR:HG22	1:E:331:CYS:H	1.68	0.58
1:A:109:MET:CE	1:A:226:LEU:HB3	2.32	0.58
1:D:330:THR:HG22	1:D:331:CYS:H	1.68	0.58
1:C:308:ARG:HH11	1:C:308:ARG:CG	2.15	0.58
1:B:45:TYR:CD2	1:B:66:LEU:HD13	2.38	0.58
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.69	0.58
1:A:94:PHE:HZ	1:I:308:ARG:CB	2.17	0.58
1:B:189:SER:HB2	1:B:213:ASN:OD1	2.04	0.58
1:C:141:GLU:O	1:E:330:THR:OG1	2.22	0.57
1:D:151:ALA:HB2	1:D:170:LEU:HG	1.85	0.57
1:A:94:PHE:HZ	1:I:308:ARG:CG	2.17	0.57
1:A:308:ARG:HH11	1:A:308:ARG:CG	2.17	0.57
1:F:330:THR:HG22	1:F:331:CYS:H	1.69	0.57
1:C:217:LYS:HE3	1:C:221:ASP:OD1	2.04	0.57
1:C:85:TYR:CE2	1:C:248:SER:HB3	2.40	0.57
1:C:94:PHE:HZ	1:H:308:ARG:HG3	1.66	0.57
1:I:151:ALA:HB2	1:I:170:LEU:HG	1.85	0.57
1:A:82:ALA:CB	1:I:256:MET:HE2	2.35	0.57
1:A:85:TYR:CE2	1:A:248:SER:HB3	2.40	0.56
1:C:82:ALA:CB	1:H:256:MET:HE2	2.36	0.56
1:I:130:ILE:HB	1:I:131:PRO:HD3	1.87	0.56
1:A:94:PHE:HZ	1:I:308:ARG:HG3	1.70	0.56
1:C:89:GLU:O	1:H:71:TYR:OH	2.22	0.56
1:B:95:TYR:CD2	1:B:206:GLU:HG3	2.41	0.56
1:C:95:TYR:CD2	1:C:206:GLU:HG3	2.40	0.56
1:H:151:ALA:HB2	1:H:170:LEU:HG	1.88	0.56
1:G:130:ILE:HB	1:G:131:PRO:HD3	1.88	0.56
1:E:326:LEU:O	1:E:327:ARG:HG3	2.06	0.56
1:C:45:TYR:CD2	1:C:66:LEU:HD13	2.41	0.55
1:C:120:THR:HG22	1:C:188:TYR:HA	1.89	0.55
1:H:130:ILE:HB	1:H:131:PRO:HD3	1.89	0.55
1:G:151:ALA:HB2	1:G:170:LEU:HG	1.88	0.55
1:C:308:ARG:NH1	1:C:308:ARG:O	2.40	0.55
1:C:141:GLU:O	1:E:330:THR:HB	2.06	0.55
1:B:120:THR:HG22	1:B:188:TYR:HA	1.87	0.55
1:A:50:ARG:NH1	1:A:50:ARG:HG3	2.21	0.54
1:B:109:MET:CE	1:B:226:LEU:HB3	2.35	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:317:TYR:CE2	1:I:4:LYS:HE2	2.42	0.54
1:D:206:GLU:OE1	4:D:607:HOH:O	2.18	0.54
1:C:109:MET:CE	1:C:226:LEU:HB3	2.37	0.54
1:A:120:THR:HG22	1:A:188:TYR:HA	1.88	0.54
1:B:50:ARG:HH11	1:B:50:ARG:HG3	1.72	0.54
1:B:308:ARG:O	1:B:308:ARG:NH1	2.40	0.54
1:F:63:ASP:HA	1:F:249:HIS:CD2	2.43	0.54
1:D:326:LEU:O	1:D:327:ARG:HG3	2.07	0.54
1:C:26:MET:O	1:C:30:ILE:HB	2.07	0.54
1:A:191:ALA:O	1:A:194:CYS:HB3	2.08	0.54
1:B:29:VAL:HG12	1:B:30:ILE:HD12	1.89	0.53
1:C:29:VAL:HG12	1:C:30:ILE:HD12	1.90	0.53
1:A:45:TYR:CD2	1:A:66:LEU:HD13	2.44	0.53
1:C:23:ARG:HA	1:C:37:VAL:HG12	1.91	0.52
1:B:26:MET:O	1:B:30:ILE:HB	2.09	0.52
1:B:50:ARG:NH1	1:B:50:ARG:HG3	2.23	0.52
1:G:326:LEU:O	1:G:327:ARG:HG3	2.10	0.52
1:I:326:LEU:O	1:I:327:ARG:HG3	2.09	0.52
1:D:117:SER:OG	1:D:157:SER:HB3	2.08	0.52
1:C:191:ALA:O	1:C:194:CYS:HB3	2.10	0.52
1:I:85:TYR:HE2	1:I:248:SER:HB3	1.74	0.52
1:E:85:TYR:HE2	1:E:248:SER:HB3	1.74	0.52
1:E:63:ASP:HA	1:E:249:HIS:CD2	2.44	0.51
1:A:82:ALA:CB	1:I:256:MET:HE1	2.33	0.51
1:B:191:ALA:O	1:B:194:CYS:HB3	2.11	0.51
1:H:326:LEU:O	1:H:327:ARG:HG3	2.11	0.51
1:A:23:ARG:HA	1:A:37:VAL:HG12	1.90	0.51
1:H:85:TYR:HE2	1:H:248:SER:HB3	1.75	0.51
1:D:189:SER:HB2	1:D:213:ASN:OD1	2.11	0.51
1:A:29:VAL:HG12	1:A:30:ILE:HD12	1.92	0.51
1:C:50:ARG:HH11	1:C:50:ARG:HG3	1.76	0.51
1:E:189:SER:HB2	1:E:213:ASN:OD1	2.11	0.50
1:B:45:TYR:CE2	1:B:66:LEU:HD13	2.45	0.50
1:A:26:MET:O	1:A:30:ILE:HB	2.11	0.50
1:H:206:GLU:HG2	1:H:208:SER:H	1.76	0.50
1:C:326:LEU:HG	1:C:326:LEU:O	2.12	0.50
1:I:206:GLU:HG2	1:I:208:SER:H	1.77	0.50
1:B:23:ARG:HA	1:B:37:VAL:HG12	1.93	0.50
1:F:326:LEU:O	1:F:327:ARG:HG3	2.11	0.50
1:E:117:SER:OG	1:E:157:SER:HB3	2.12	0.49
1:C:317:TYR:CE2	1:H:4:LYS:HE2	2.47	0.49
1:D:85:TYR:HE2	1:D:248:SER:HB3	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:ARG:O	1:A:308:ARG:NH1	2.41	0.49
1:F:117:SER:OG	1:F:157:SER:HB3	2.12	0.49
1:G:85:TYR:HE2	1:G:248:SER:HB3	1.76	0.49
1:F:189:SER:HB2	1:F:213:ASN:OD1	2.13	0.49
1:F:214:LEU:CD1	1:F:219:ASP:HB2	2.42	0.49
1:B:326:LEU:O	1:B:326:LEU:HG	2.13	0.49
1:I:330:THR:HG22	1:I:331:CYS:N	2.27	0.49
1:C:50:ARG:HG3	1:C:50:ARG:NH1	2.28	0.49
1:F:85:TYR:HE2	1:F:248:SER:HB3	1.78	0.48
1:B:137:CYS:O	1:B:143:ARG:NH2	2.46	0.48
1:E:132:ILE:HG22	1:E:326:LEU:HD11	1.95	0.48
1:G:206:GLU:HG2	1:G:208:SER:H	1.78	0.48
1:C:45:TYR:CE2	1:C:66:LEU:HD13	2.48	0.48
1:H:85:TYR:HE2	1:H:248:SER:CB	2.27	0.48
1:D:63:ASP:HA	1:D:249:HIS:CD2	2.49	0.48
1:G:71:TYR:HB2	1:G:311:ALA:CB	2.43	0.48
1:A:108:GLN:NE2	1:A:232:ARG:HG3	2.21	0.48
1:E:214:LEU:CD1	1:E:219:ASP:HB2	2.43	0.48
1:H:330:THR:HG22	1:H:331:CYS:N	2.26	0.47
1:A:107:PHE:CB	1:A:115:LYS:HE3	2.43	0.47
1:B:115:LYS:O	1:B:154:PHE:HB3	2.15	0.47
1:B:85:TYR:CE2	1:B:248:SER:HB3	2.48	0.47
1:A:326:LEU:HG	1:A:326:LEU:O	2.13	0.47
1:D:206:GLU:HG2	1:D:208:SER:H	1.80	0.47
1:H:78:LYS:HA	1:H:78:LYS:HD3	1.73	0.47
1:C:107:PHE:CB	1:C:115:LYS:HE3	2.43	0.47
1:G:78:LYS:HD3	1:G:78:LYS:HA	1.73	0.47
1:D:78:LYS:HD3	1:D:78:LYS:HA	1.72	0.47
1:H:214:LEU:CD1	1:H:219:ASP:HB2	2.45	0.47
1:A:85:TYR:HE2	1:A:248:SER:HB3	1.80	0.47
1:C:133:GLY:HA2	1:C:326:LEU:HD13	1.96	0.46
1:C:137:CYS:O	1:C:143:ARG:NH2	2.47	0.46
1:E:186:PHE:O	1:E:190:GLY:HA3	2.15	0.46
1:D:214:LEU:CD1	1:D:219:ASP:HB2	2.42	0.46
1:B:199:ALA:HA	1:F:13:GLU:HG3	1.96	0.46
1:C:73:ALA:HA	1:C:76:ASN:OD1	2.16	0.46
1:I:71:TYR:HB2	1:I:311:ALA:CB	2.45	0.46
1:B:107:PHE:CB	1:B:115:LYS:HE3	2.43	0.46
1:G:224:GLU:OE2	1:G:232:ARG:HD3	2.15	0.46
1:B:108:GLN:H	1:B:111:GLN:HG3	1.81	0.45
1:G:132:ILE:HG22	1:G:326:LEU:HD11	1.98	0.45
1:H:71:TYR:HB2	1:H:311:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:324:ARG:C	1:B:326:LEU:H	2.19	0.45
1:B:157:SER:HA	1:B:173:LEU:HD22	1.99	0.45
1:A:176:GLY:HA3	1:D:176:GLY:HA3	1.98	0.45
1:I:189:SER:HB2	1:I:213:ASN:OD1	2.16	0.45
1:E:78:LYS:HA	1:E:78:LYS:HD3	1.71	0.45
1:A:115:LYS:O	1:A:154:PHE:HB3	2.16	0.45
1:F:206:GLU:HG2	1:F:208:SER:H	1.80	0.45
1:A:133:GLY:HA2	1:A:326:LEU:HD13	1.98	0.45
1:E:268:ASN:O	1:E:271:GLN:HB3	2.16	0.45
1:A:120:THR:OG1	1:A:127:GLY:HA3	2.17	0.45
1:I:85:TYR:HE2	1:I:248:SER:CB	2.30	0.45
1:E:206:GLU:HG2	1:E:208:SER:H	1.82	0.45
1:B:133:GLY:HA2	1:B:326:LEU:HD13	1.99	0.45
1:G:117:SER:OG	1:G:157:SER:HB3	2.16	0.45
1:I:78:LYS:HA	1:I:78:LYS:HD3	1.75	0.45
1:F:157:SER:HA	1:F:173:LEU:HD22	1.99	0.44
1:C:68:TYR:HB2	1:C:315:LEU:HD11	1.99	0.44
1:G:214:LEU:CD1	1:G:219:ASP:HB2	2.48	0.44
1:G:189:SER:HB2	1:G:213:ASN:OD1	2.17	0.44
1:C:94:PHE:CZ	1:H:308:ARG:CB	2.94	0.44
1:I:132:ILE:HG22	1:I:326:LEU:HD11	1.98	0.44
1:F:186:PHE:O	1:F:190:GLY:HA3	2.18	0.44
1:C:330:THR:HG22	1:C:331:CYS:N	2.29	0.44
1:G:85:TYR:HE2	1:G:248:SER:CB	2.31	0.44
1:I:214:LEU:CD1	1:I:219:ASP:HB2	2.47	0.44
1:B:280:LYS:C	1:B:283:GLN:HE22	2.20	0.44
1:A:137:CYS:O	1:A:143:ARG:NH2	2.50	0.44
1:A:199:ALA:HA	1:D:13:GLU:HG3	1.99	0.44
1:A:108:GLN:H	1:A:111:GLN:HG3	1.83	0.44
1:B:276:LYS:O	1:B:278:LYS:HD2	2.17	0.44
1:G:330:THR:HG22	1:G:331:CYS:N	2.28	0.44
1:C:261:ASP:CG	1:F:317:TYR:HB3	2.37	0.44
1:D:157:SER:HA	1:D:173:LEU:HD22	2.00	0.43
1:A:68:TYR:HB2	1:A:315:LEU:HD11	2.00	0.43
1:A:89:GLU:HG2	1:F:272:GLU:OE1	2.18	0.43
1:F:132:ILE:HG22	1:F:326:LEU:HD11	1.99	0.43
1:C:324:ARG:C	1:C:326:LEU:H	2.21	0.43
1:A:131:PRO:HB3	1:A:204:PHE:CD1	2.53	0.43
1:C:115:LYS:O	1:C:154:PHE:HB3	2.17	0.43
1:A:73:ALA:HA	1:A:76:ASN:OD1	2.19	0.43
1:B:131:PRO:HB3	1:B:204:PHE:CD1	2.54	0.43
1:C:108:GLN:H	1:C:111:GLN:HG3	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:120:THR:OG1	1:C:127:GLY:HA3	2.19	0.43
1:H:117:SER:OG	1:H:157:SER:HB3	2.18	0.43
1:F:280:LYS:HD3	1:F:280:LYS:HA	1.80	0.43
1:F:78:LYS:HA	1:F:78:LYS:HD3	1.73	0.43
1:C:85:TYR:HE2	1:C:248:SER:HB3	1.84	0.43
1:C:76:ASN:N	1:C:76:ASN:OD1	2.49	0.43
1:I:117:SER:OG	1:I:157:SER:HB3	2.18	0.43
1:G:157:SER:HA	1:G:173:LEU:HD22	2.00	0.43
1:C:94:PHE:CD2	1:C:94:PHE:C	2.92	0.43
1:A:45:TYR:CE2	1:A:66:LEU:HD13	2.53	0.43
1:H:189:SER:HB2	1:H:213:ASN:OD1	2.18	0.43
1:G:330:THR:CG2	1:G:331:CYS:H	2.26	0.43
1:H:132:ILE:HG22	1:H:326:LEU:HD11	2.01	0.43
1:C:131:PRO:HB3	1:C:204:PHE:CD1	2.53	0.43
1:A:261:ASP:CG	1:E:317:TYR:HB3	2.39	0.42
1:A:324:ARG:C	1:A:326:LEU:H	2.22	0.42
1:A:276:LYS:O	1:A:278:LYS:HD2	2.19	0.42
1:D:58:ASP:OD1	1:D:254:ARG:NH2	2.53	0.42
1:B:73:ALA:HA	1:B:76:ASN:OD1	2.19	0.42
1:D:132:ILE:HG22	1:D:326:LEU:HD11	2.00	0.42
1:H:120:THR:OG1	1:H:127:GLY:HA3	2.19	0.42
1:A:277:ASP:OD2	1:F:88:LYS:HG3	2.19	0.42
1:B:220:ARG:C	1:B:222:GLN:H	2.23	0.42
1:B:330:THR:HG22	1:B:331:CYS:N	2.27	0.42
1:A:280:LYS:C	1:A:283:GLN:HE22	2.23	0.42
1:H:224:GLU:OE2	1:H:232:ARG:HD3	2.20	0.42
1:C:82:ALA:CB	1:H:256:MET:HE1	2.38	0.42
1:C:63:ASP:HA	1:C:249:HIS:CG	2.55	0.42
1:E:157:SER:HA	1:E:173:LEU:HD22	2.01	0.42
1:B:186:PHE:O	1:B:190:GLY:HA3	2.20	0.42
1:B:120:THR:OG1	1:B:127:GLY:HA3	2.20	0.42
1:A:330:THR:HG22	1:A:331:CYS:N	2.30	0.41
1:A:130:ILE:HB	1:A:131:PRO:CD	2.49	0.41
1:B:176:GLY:HA3	1:F:176:GLY:HA3	2.01	0.41
1:G:45:TYR:CZ	1:G:66:LEU:HD22	2.55	0.41
1:G:120:THR:OG1	1:G:127:GLY:HA3	2.20	0.41
1:B:144:LYS:NZ	1:B:328:GLU:OE2	2.53	0.41
1:A:76:ASN:OD1	1:A:76:ASN:N	2.53	0.41
1:H:157:SER:HA	1:H:173:LEU:HD22	2.01	0.41
1:C:280:LYS:C	1:C:283:GLN:HE22	2.23	0.41
1:I:127:GLY:N	3:I:600:CO3:O1	2.51	0.41
1:C:261:ASP:CG	1:F:317:TYR:CB	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:276:LYS:O	1:C:278:LYS:HD2	2.20	0.41
1:G:280:LYS:HA	1:G:280:LYS:HD3	1.85	0.41
1:C:144:LYS:NZ	1:C:328:GLU:OE2	2.52	0.41
1:B:279:SER:O	1:B:283:GLN:NE2	2.54	0.41
1:B:76:ASN:OD1	1:B:76:ASN:N	2.54	0.41
1:D:280:LYS:HD3	1:D:280:LYS:HA	1.80	0.41
1:D:45:TYR:CZ	1:D:66:LEU:HD22	2.56	0.41
1:E:246:VAL:HA	1:E:247:PRO:HD3	1.95	0.41
1:H:280:LYS:HD3	1:H:280:LYS:HA	1.85	0.41
1:D:186:PHE:O	1:D:190:GLY:HA3	2.21	0.41
1:A:279:SER:O	1:A:283:GLN:NE2	2.54	0.40
1:C:254:ARG:NH1	1:C:257:GLY:O	2.54	0.40
1:B:99:ALA:HB3	1:B:226:LEU:HB2	2.02	0.40
1:E:63:ASP:HB2	1:E:249:HIS:CE1	2.57	0.40
1:C:157:SER:HA	1:C:173:LEU:HD22	2.02	0.40
1:C:276:LYS:NZ	1:C:299:ALA:O	2.45	0.40
1:A:90:ASP:OD1	1:I:310:ASP:CB	2.69	0.40
1:I:311:ALA:O	1:I:315:LEU:HG	2.22	0.40
1:B:277:ASP:OD2	1:D:88:LYS:HG3	2.22	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	Distance(Å)	Clash(Å)
1:A:141:GLU:O	1:F:330:THR:OG1[3_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	327/337 (97%)	289 (88%)	33 (10%)	5 (2%)	15	46
1	B	327/337 (97%)	288 (88%)	35 (11%)	4 (1%)	19	54
1	C	327/337 (97%)	289 (88%)	33 (10%)	5 (2%)	15	46
1	D	327/337 (97%)	302 (92%)	25 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	327/337 (97%)	302 (92%)	25 (8%)	0	100	100
1	F	327/337 (97%)	302 (92%)	25 (8%)	0	100	100
1	G	327/337 (97%)	300 (92%)	27 (8%)	0	100	100
1	H	327/337 (97%)	303 (93%)	24 (7%)	0	100	100
1	I	327/337 (97%)	301 (92%)	26 (8%)	0	100	100
All	All	2943/3033 (97%)	2676 (91%)	253 (9%)	14 (0%)	38	76

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	GLU
1	C	281	GLU
1	B	12	SER
1	B	277	ASP
1	B	330	THR
1	A	281	GLU
1	C	12	SER
1	C	277	ASP
1	C	330	THR
1	A	12	SER
1	A	325	ASN
1	A	330	THR
1	A	277	ASP
1	C	325	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/281 (98%)	256 (93%)	18 (7%)	24	56
1	B	274/281 (98%)	257 (94%)	17 (6%)	26	60
1	C	274/281 (98%)	257 (94%)	17 (6%)	26	60
1	D	274/281 (98%)	262 (96%)	12 (4%)	39	75
1	E	274/281 (98%)	261 (95%)	13 (5%)	36	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	274/281 (98%)	262 (96%)	12 (4%)	39	75
1	G	274/281 (98%)	261 (95%)	13 (5%)	36	73
1	H	274/281 (98%)	261 (95%)	13 (5%)	36	73
1	I	274/281 (98%)	260 (95%)	14 (5%)	33	69
All	All	2466/2529 (98%)	2337 (95%)	129 (5%)	32	68

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	VAL
1	B	71	TYR
1	B	76	ASN
1	B	80	VAL
1	B	135	LEU
1	B	165	THR
1	B	182	LEU
1	B	206	GLU
1	B	216	ASN
1	B	217	LYS
1	B	226	LEU
1	B	261	ASP
1	B	262	LEU
1	B	278	LYS
1	B	279	SER
1	B	308	ARG
1	B	318	GLU
1	A	29	VAL
1	A	71	TYR
1	A	76	ASN
1	A	80	VAL
1	A	135	LEU
1	A	165	THR
1	A	182	LEU
1	A	205	VAL
1	A	206	GLU
1	A	216	ASN
1	A	217	LYS
1	A	226	LEU
1	A	261	ASP
1	A	262	LEU
1	A	278	LYS

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Mol	Chain	Res	Type
1	A	279	SER
1	A	308	ARG
1	A	318	GLU
1	C	29	VAL
1	C	71	TYR
1	C	76	ASN
1	C	80	VAL
1	C	135	LEU
1	C	165	THR
1	C	182	LEU
1	C	206	GLU
1	C	216	ASN
1	C	217	LYS
1	C	226	LEU
1	C	261	ASP
1	C	262	LEU
1	C	278	LYS
1	C	279	SER
1	C	308	ARG
1	C	318	GLU
1	D	12	SER
1	D	63	ASP
1	D	135	LEU
1	D	173	LEU
1	D	207	HIS
1	D	214	LEU
1	D	226	LEU
1	D	262	LEU
1	D	283	GLN
1	D	318	GLU
1	D	328	GLU
1	D	330	THR
1	E	12	SER
1	E	63	ASP
1	E	135	LEU
1	E	138	ASP
1	E	173	LEU
1	E	207	HIS
1	E	214	LEU
1	E	226	LEU
1	E	262	LEU
1	E	283	GLN

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Mol	Chain	Res	Type
1	E	318	GLU
1	E	328	GLU
1	E	330	THR
1	F	12	SER
1	F	63	ASP
1	F	135	LEU
1	F	173	LEU
1	F	207	HIS
1	F	214	LEU
1	F	226	LEU
1	F	262	LEU
1	F	283	GLN
1	F	318	GLU
1	F	328	GLU
1	F	330	THR
1	G	12	SER
1	G	63	ASP
1	G	135	LEU
1	G	173	LEU
1	G	207	HIS
1	G	214	LEU
1	G	226	LEU
1	G	260	GLU
1	G	262	LEU
1	G	283	GLN
1	G	318	GLU
1	G	328	GLU
1	G	330	THR
1	H	12	SER
1	H	63	ASP
1	H	135	LEU
1	H	173	LEU
1	H	207	HIS
1	H	214	LEU
1	H	226	LEU
1	H	260	GLU
1	H	262	LEU
1	H	283	GLN
1	H	318	GLU
1	H	328	GLU
1	H	330	THR
1	I	12	SER

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Mol	Chain	Res	Type
1	I	63	ASP
1	I	135	LEU
1	I	173	LEU
1	I	189	SER
1	I	207	HIS
1	I	214	LEU
1	I	226	LEU
1	I	260	GLU
1	I	262	LEU
1	I	283	GLN
1	I	318	GLU
1	I	328	GLU
1	I	330	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	GLN
1	B	283	GLN
1	B	325	ASN
1	A	108	GLN
1	A	283	GLN
1	A	325	ASN
1	C	283	GLN
1	C	325	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	CO3	A	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	B	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	C	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	D	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	E	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	F	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	G	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	H	600	2	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	I	600	2	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CO3	A	600	2	-	0/0/0/0	0/0/0/0
3	CO3	B	600	2	-	0/0/0/0	0/0/0/0
3	CO3	C	600	2	-	0/0/0/0	0/0/0/0
3	CO3	D	600	2	-	0/0/0/0	0/0/0/0
3	CO3	E	600	2	-	0/0/0/0	0/0/0/0
3	CO3	F	600	2	-	0/0/0/0	0/0/0/0
3	CO3	G	600	2	-	0/0/0/0	0/0/0/0
3	CO3	H	600	2	-	0/0/0/0	0/0/0/0
3	CO3	I	600	2	-	0/0/0/0	0/0/0/0

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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/337 (97%)	2.35	190 (57%) 0 0	48, 57, 64, 69	0
1	B	329/337 (97%)	2.55	205 (62%) 0 0	48, 57, 64, 70	0
1	C	329/337 (97%)	0.45	5 (1%) 70 71	48, 57, 64, 70	0
1	D	329/337 (97%)	0.70	30 (9%) 9 8	47, 57, 64, 70	0
1	E	329/337 (97%)	0.58	27 (8%) 12 10	47, 57, 64, 70	0
1	F	329/337 (97%)	0.56	23 (6%) 16 14	47, 57, 64, 70	0
1	G	329/337 (97%)	0.83	41 (12%) 5 4	47, 57, 64, 70	0
1	H	329/337 (97%)	0.73	40 (12%) 5 4	47, 57, 64, 70	0
1	I	329/337 (97%)	0.72	28 (8%) 11 9	47, 57, 64, 70	0
All	All	2961/3033 (97%)	1.05	589 (19%) 2 1	47, 57, 64, 70	0

All (589) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	MET	9.0
1	A	256	MET	8.3
1	D	139	LEU	7.8
1	D	330	THR	7.6
1	F	331	CYS	7.6
1	A	257	GLY	7.2
1	A	80	VAL	6.8
1	A	81	VAL	6.5
1	D	90	ASP	6.4
1	B	257	GLY	6.3
1	G	142	PRO	6.2
1	B	331	CYS	6.0
1	A	59	ALA	6.0
1	B	307	PRO	6.0
1	B	139	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	30	ILE	5.7
1	B	179	CYS	5.7
1	B	37	VAL	5.7
1	B	252	VAL	5.6
1	B	49	ILE	5.6
1	G	138	ASP	5.6
1	B	32	SER	5.5
1	I	146	LEU	5.4
1	E	256	MET	5.4
1	F	330	THR	5.3
1	B	167	PHE	5.3
1	B	6	VAL	5.2
1	E	86	GLY	5.1
1	B	30	ILE	5.1
1	B	328	GLU	5.1
1	H	311	ALA	5.0
1	I	308	ARG	5.0
1	A	307	PRO	5.0
1	D	308	ARG	5.0
1	E	330	THR	4.9
1	E	140	PRO	4.9
1	A	314	TYR	4.9
1	F	139	LEU	4.9
1	B	306	PRO	4.9
1	B	3	ASP	4.9
1	D	328	GLU	4.9
1	B	79	PRO	4.9
1	B	48	CYS	4.8
1	F	140	PRO	4.8
1	A	306	PRO	4.8
1	E	226	LEU	4.8
1	D	331	CYS	4.8
1	B	204	PHE	4.8
1	B	311	ALA	4.8
1	B	308	ARG	4.7
1	B	39	CYS	4.7
1	B	59	ALA	4.7
1	A	255	SER	4.7
1	F	89	GLU	4.7
1	B	255	SER	4.7
1	B	107	PHE	4.7
1	D	140	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	4.6
1	H	167	PHE	4.6
1	A	39	CYS	4.6
1	I	33	ASP	4.6
1	B	54	ALA	4.6
1	E	322	ALA	4.6
1	B	61	THR	4.6
1	A	145	PRO	4.6
1	A	252	VAL	4.6
1	B	146	LEU	4.5
1	B	285	PHE	4.5
1	A	139	LEU	4.5
1	B	43	ALA	4.5
1	A	79	PRO	4.5
1	H	308	ARG	4.5
1	G	143	ARG	4.4
1	B	31	PRO	4.4
1	A	33	ASP	4.4
1	A	5	THR	4.4
1	E	142	PRO	4.4
1	A	262	LEU	4.4
1	A	37	VAL	4.4
1	B	262	LEU	4.4
1	A	136	TYR	4.3
1	A	309	MET	4.3
1	A	199	ALA	4.3
1	A	316	GLY	4.3
1	A	131	PRO	4.3
1	D	104	ASP	4.3
1	B	77	LEU	4.3
1	E	139	LEU	4.3
1	A	180	SER	4.2
1	D	325	ASN	4.2
1	A	60	VAL	4.2
1	A	179	CYS	4.2
1	D	142	PRO	4.2
1	A	71	TYR	4.2
1	A	261	ASP	4.2
1	A	315	LEU	4.2
1	B	68	TYR	4.2
1	H	235	VAL	4.2
1	A	14	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	4.2
1	A	251	VAL	4.1
1	I	91	PRO	4.1
1	B	315	LEU	4.1
1	B	161	CYS	4.1
1	A	65	GLY	4.1
1	B	33	ASP	4.1
1	B	207	HIS	4.0
1	B	74	PRO	4.0
1	B	317	TYR	4.0
1	B	261	ASP	4.0
1	B	5	THR	4.0
1	H	281	GLU	4.0
1	B	326	LEU	4.0
1	A	331	CYS	4.0
1	D	200	GLY	4.0
1	G	33	ASP	3.9
1	F	90	ASP	3.9
1	A	244	ALA	3.9
1	B	36	SER	3.9
1	B	266	LEU	3.9
1	I	34	GLY	3.9
1	A	3	ASP	3.9
1	A	317	TYR	3.8
1	A	168	PRO	3.8
1	A	7	ARG	3.8
1	E	331	CYS	3.8
1	A	146	LEU	3.8
1	B	180	SER	3.8
1	A	32	SER	3.8
1	A	72	LEU	3.8
1	B	302	PHE	3.8
1	F	317	TYR	3.8
1	A	308	ARG	3.8
1	A	243	LEU	3.8
1	G	104	ASP	3.7
1	B	213	ASN	3.7
1	B	145	PRO	3.7
1	B	246	VAL	3.7
1	A	286	SER	3.7
1	B	319	TYR	3.7
1	B	314	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	40	VAL	3.7
1	B	67	VAL	3.7
1	F	75	ASN	3.7
1	G	166	ASP	3.7
1	B	122	LEU	3.7
1	A	258	GLY	3.7
1	B	154	PHE	3.7
1	G	306	PRO	3.7
1	B	9	CYS	3.6
1	D	138	ASP	3.6
1	E	90	ASP	3.6
1	E	325	ASN	3.6
1	B	263	ILE	3.6
1	B	55	ASN	3.6
1	B	51	ALA	3.6
1	A	43	ALA	3.6
1	F	308	ARG	3.6
1	B	7	ARG	3.5
1	B	81	VAL	3.5
1	B	64	ALA	3.5
1	A	31	PRO	3.5
1	A	125	SER	3.5
1	A	142	PRO	3.5
1	B	132	ILE	3.5
1	B	141	GLU	3.5
1	A	74	PRO	3.5
1	B	121	GLY	3.5
1	A	55	ASN	3.5
1	B	273	HIS	3.5
1	B	58	ASP	3.5
1	B	227	CYS	3.5
1	B	316	GLY	3.5
1	A	36	SER	3.5
1	D	322	ALA	3.5
1	A	161	CYS	3.4
1	B	320	VAL	3.4
1	B	53	ALA	3.4
1	B	323	ILE	3.4
1	F	74	PRO	3.4
1	H	141	GLU	3.4
1	D	136	TYR	3.4
1	A	107	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	143	ARG	3.4
1	A	70	ALA	3.4
1	B	164	GLY	3.4
1	D	86	GLY	3.4
1	B	44	SER	3.4
1	A	23	ARG	3.4
1	H	313	MET	3.4
1	B	60	VAL	3.3
1	B	78	LYS	3.3
1	A	304	LYS	3.3
1	B	29	VAL	3.3
1	B	71	TYR	3.3
1	B	231	THR	3.3
1	H	265	GLU	3.3
1	H	33	ASP	3.3
1	A	260	GLU	3.3
1	B	162	ALA	3.3
1	G	307	PRO	3.3
1	B	313	MET	3.3
1	B	138	ASP	3.3
1	B	129	ASN	3.3
1	A	103	LYS	3.3
1	E	308	ARG	3.3
1	G	29	VAL	3.3
1	F	144	LYS	3.3
1	A	319	TYR	3.3
1	G	281	GLU	3.2
1	B	106	GLY	3.2
1	A	121	GLY	3.2
1	B	94	PHE	3.2
1	A	78	LYS	3.2
1	C	145	PRO	3.2
1	E	317	TYR	3.2
1	B	66	LEU	3.2
1	A	226	LEU	3.2
1	G	216	ASN	3.2
1	B	168	PRO	3.2
1	B	226	LEU	3.2
1	G	145	PRO	3.2
1	B	142	PRO	3.2
1	B	82	ALA	3.2
1	G	91	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	97	ALA	3.2
1	B	309	MET	3.2
1	A	328	GLU	3.2
1	H	331	CYS	3.2
1	B	28	SER	3.2
1	B	175	PRO	3.2
1	A	285	PHE	3.2
1	A	327	ARG	3.2
1	I	220	ARG	3.2
1	B	205	VAL	3.1
1	H	211	PHE	3.1
1	A	130	ILE	3.1
1	H	107	PHE	3.1
1	A	17	THR	3.1
1	G	106	GLY	3.1
1	D	317	TYR	3.1
1	B	244	ALA	3.1
1	D	256	MET	3.1
1	A	141	GLU	3.1
1	G	267	LEU	3.1
1	E	321	THR	3.1
1	B	305	VAL	3.1
1	A	126	ALA	3.1
1	B	80	VAL	3.1
1	A	29	VAL	3.1
1	A	58	ASP	3.1
1	A	302	PHE	3.0
1	A	8	TRP	3.0
1	H	146	LEU	3.0
1	A	69	ASP	3.0
1	A	181	THR	3.0
1	F	3	ASP	3.0
1	B	8	TRP	3.0
1	A	99	ALA	3.0
1	I	321	THR	3.0
1	H	182	LEU	3.0
1	A	49	ILE	3.0
1	A	227	CYS	3.0
1	B	93	THR	3.0
1	B	178	GLY	3.0
1	A	13	GLU	3.0
1	B	11	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	6	VAL	3.0
1	B	250	THR	3.0
1	A	50	ARG	3.0
1	I	330	THR	3.0
1	H	323	ILE	3.0
1	G	311	ALA	3.0
1	B	136	TYR	3.0
1	B	50	ARG	3.0
1	A	228	LEU	3.0
1	B	88	LYS	3.0
1	I	6	VAL	2.9
1	B	42	LYS	2.9
1	I	312	LYS	2.9
1	B	10	ALA	2.9
1	I	59	ALA	2.9
1	A	93	THR	2.9
1	A	120	THR	2.9
1	A	137	CYS	2.9
1	B	304	LYS	2.9
1	H	166	ASP	2.9
1	B	239	LYS	2.9
1	A	61	THR	2.9
1	B	187	GLY	2.9
1	A	176	GLY	2.9
1	B	310	ASP	2.9
1	G	282	PHE	2.9
1	G	330	THR	2.9
1	B	4	LYS	2.9
1	E	87	SER	2.9
1	B	19	CYS	2.9
1	B	12	SER	2.9
1	A	124	ARG	2.9
1	F	318	GLU	2.9
1	A	27	LYS	2.9
1	B	160	PRO	2.8
1	D	145	PRO	2.8
1	A	48	CYS	2.8
1	H	300	HIS	2.8
1	A	275	GLY	2.8
1	B	199	ALA	2.8
1	A	162	ALA	2.8
1	A	267	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	2.8
1	B	75	ASN	2.8
1	B	76	ASN	2.8
1	A	300	HIS	2.8
1	G	32	SER	2.8
1	H	71	TYR	2.8
1	D	144	LYS	2.8
1	G	214	LEU	2.8
1	B	277	ASP	2.8
1	B	258	GLY	2.8
1	A	11	VAL	2.8
1	A	299	ALA	2.8
1	B	264	TRP	2.8
1	C	215	ALA	2.8
1	A	165	THR	2.7
1	D	164	GLY	2.7
1	G	176	GLY	2.7
1	B	120	THR	2.7
1	B	170	LEU	2.7
1	B	70	ALA	2.7
1	B	126	ALA	2.7
1	A	270	ALA	2.7
1	B	251	VAL	2.7
1	A	87	SER	2.7
1	H	143	ARG	2.7
1	A	283	GLN	2.7
1	B	254	ARG	2.7
1	B	303	LEU	2.7
1	A	175	PRO	2.7
1	A	284	LEU	2.7
1	B	159	ALA	2.7
1	D	113	ARG	2.7
1	A	231	THR	2.7
1	B	85	TYR	2.7
1	B	169	GLN	2.7
1	B	270	ALA	2.7
1	A	274	PHE	2.7
1	A	19	CYS	2.7
1	A	254	ARG	2.7
1	B	21	SER	2.7
1	B	20	GLN	2.7
1	B	166	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	54	ALA	2.7
1	I	143	ARG	2.7
1	A	294	LEU	2.6
1	B	47	ASP	2.6
1	B	45	TYR	2.6
1	A	53	ALA	2.6
1	A	253	ALA	2.6
1	B	184	GLN	2.6
1	A	246	VAL	2.6
1	D	143	ARG	2.6
1	A	259	LYS	2.6
1	B	25	HIS	2.6
1	B	156	GLY	2.6
1	B	243	LEU	2.6
1	I	284	LEU	2.6
1	A	282	PHE	2.6
1	B	163	ASP	2.6
1	H	142	PRO	2.6
1	A	313	MET	2.6
1	H	147	GLU	2.6
1	A	38	ALA	2.6
1	B	46	LEU	2.6
1	B	144	LYS	2.6
1	H	79	PRO	2.6
1	A	159	ALA	2.6
1	A	86	GLY	2.6
1	A	303	LEU	2.6
1	A	40	VAL	2.6
1	A	42	LYS	2.6
1	B	283	GLN	2.6
1	B	153	PHE	2.6
1	A	52	ILE	2.6
1	B	128	TRP	2.5
1	B	260	GLU	2.5
1	A	247	PRO	2.5
1	B	267	LEU	2.5
1	B	238	TYR	2.5
1	A	311	ALA	2.5
1	A	94	PHE	2.5
1	A	263	ILE	2.5
1	B	140	PRO	2.5
1	A	66	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	134	LEU	2.5
1	A	326	LEU	2.5
1	B	300	HIS	2.5
1	A	67	VAL	2.5
1	H	277	ASP	2.5
1	A	46	LEU	2.5
1	I	214	LEU	2.5
1	B	247	PRO	2.5
1	B	26	MET	2.5
1	A	188	TYR	2.5
1	A	44	SER	2.5
1	F	226	LEU	2.5
1	A	118	CYS	2.5
1	A	154	PHE	2.5
1	F	322	ALA	2.5
1	B	327	ARG	2.5
1	H	278	LYS	2.5
1	B	35	PRO	2.5
1	B	99	ALA	2.5
1	A	242	HIS	2.4
1	H	91	PRO	2.4
1	B	274	PHE	2.4
1	I	216	ASN	2.4
1	I	32	SER	2.4
1	A	295	PHE	2.4
1	A	98	VAL	2.4
1	E	37	VAL	2.4
1	C	331	CYS	2.4
1	G	31	PRO	2.4
1	G	141	GLU	2.4
1	G	312	LYS	2.4
1	B	14	HIS	2.4
1	F	256	MET	2.4
1	A	293	LEU	2.4
1	B	321	THR	2.4
1	A	312	LYS	2.4
1	B	158	CYS	2.4
1	I	320	VAL	2.4
1	A	20	GLN	2.4
1	I	28	SER	2.4
1	I	92	GLN	2.4
1	A	10	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	264	TRP	2.4
1	G	86	GLY	2.4
1	G	146	LEU	2.4
1	G	315	LEU	2.4
1	B	92	GLN	2.4
1	B	52	ILE	2.4
1	B	182	LEU	2.4
1	G	331	CYS	2.4
1	B	86	GLY	2.4
1	A	21	SER	2.4
1	H	258	GLY	2.4
1	B	289	HIS	2.4
1	G	283	GLN	2.3
1	A	104	ASP	2.3
1	E	77	LEU	2.3
1	F	71	TYR	2.3
1	A	167	PHE	2.3
1	E	106	GLY	2.3
1	A	273	HIS	2.3
1	D	103	LYS	2.3
1	B	109	MET	2.3
1	I	283	GLN	2.3
1	A	4	LYS	2.3
1	A	119	HIS	2.3
1	G	30	ILE	2.3
1	A	26	MET	2.3
1	G	82	ALA	2.3
1	B	83	GLU	2.3
1	A	183	ASN	2.3
1	A	213	ASN	2.3
1	B	294	LEU	2.3
1	H	315	LEU	2.3
1	A	205	VAL	2.3
1	A	25	HIS	2.3
1	E	89	GLU	2.3
1	I	22	PHE	2.3
1	B	284	LEU	2.3
1	D	172	GLN	2.3
1	A	123	GLY	2.3
1	A	230	ASN	2.3
1	B	157	SER	2.3
1	E	323	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	65	GLY	2.3
1	A	9	CYS	2.3
1	A	85	TYR	2.3
1	A	189	SER	2.2
1	A	76	ASN	2.2
1	B	135	LEU	2.2
1	C	139	LEU	2.2
1	F	127	GLY	2.2
1	H	34	GLY	2.2
1	I	309	MET	2.2
1	A	22	PHE	2.2
1	G	317	TYR	2.2
1	I	5	THR	2.2
1	B	297	ASP	2.2
1	F	219	ASP	2.2
1	G	286	SER	2.2
1	A	82	ALA	2.2
1	A	73	ALA	2.2
1	B	188	TYR	2.2
1	B	229	ASP	2.2
1	H	309	MET	2.2
1	B	73	ALA	2.2
1	A	41	LYS	2.2
1	E	218	ALA	2.2
1	H	99	ALA	2.2
1	A	182	LEU	2.2
1	E	319	TYR	2.2
1	F	68	TYR	2.2
1	A	47	ASP	2.2
1	A	166	ASP	2.2
1	D	3	ASP	2.2
1	D	250	THR	2.2
1	G	258	GLY	2.2
1	H	330	THR	2.2
1	H	25	HIS	2.2
1	B	117	SER	2.2
1	B	22	PHE	2.2
1	A	109	MET	2.2
1	H	59	ALA	2.2
1	H	137	CYS	2.2
1	F	165	THR	2.2
1	A	116	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	192	PHE	2.2
1	E	107	PHE	2.2
1	A	169	GLN	2.2
1	F	143	ARG	2.2
1	G	287	SER	2.1
1	I	269	GLN	2.1
1	D	89	GLU	2.1
1	B	95	TYR	2.1
1	A	68	TYR	2.1
1	A	238	TYR	2.1
1	A	292	ASP	2.1
1	A	310	ASP	2.1
1	C	327	ARG	2.1
1	H	165	THR	2.1
1	B	131	PRO	2.1
1	G	74	PRO	2.1
1	G	175	PRO	2.1
1	B	293	LEU	2.1
1	B	190	GLY	2.1
1	A	96	TYR	2.1
1	G	316	GLY	2.1
1	B	172	GLN	2.1
1	G	280	LYS	2.1
1	H	26	MET	2.1
1	G	37	VAL	2.1
1	H	305	VAL	2.1
1	B	69	ASP	2.1
1	B	198	GLY	2.1
1	D	74	PRO	2.1
1	D	106	GLY	2.1
1	A	97	ALA	2.1
1	A	218	ALA	2.1
1	H	38	ALA	2.1
1	B	281	GLU	2.1
1	A	132	ILE	2.1
1	B	269	GLN	2.1
1	I	230	ASN	2.1
1	B	295	PHE	2.1
1	E	78	LYS	2.1
1	B	203	ALA	2.1
1	A	45	TYR	2.1
1	B	280	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	137	CYS	2.1
1	B	87	SER	2.1
1	B	189	SER	2.1
1	A	62	LEU	2.1
1	A	301	GLY	2.1
1	F	235	VAL	2.1
1	B	130	ILE	2.1
1	G	264	TRP	2.1
1	B	112	LEU	2.1
1	E	326	LEU	2.1
1	A	28	SER	2.1
1	H	109	MET	2.0
1	E	71	TYR	2.0
1	B	268	ASN	2.0
1	A	129	ASN	2.0
1	D	318	GLU	2.0
1	I	300	HIS	2.0
1	A	277	ASP	2.0
1	I	23	ARG	2.0
1	A	91	PRO	2.0
1	H	145	PRO	2.0
1	B	149	ALA	2.0
1	B	278	LYS	2.0
1	A	148	LYS	2.0
1	A	276	LYS	2.0
1	B	91	PRO	2.0
1	B	150	VAL	2.0
1	E	312	LYS	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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CO3	F	600	4/4	0.23	0.39	49,49,50,50	0
3	CO3	E	600	4/4	0.18	-0.11	49,49,50,50	0
3	CO3	D	600	4/4	0.15	-0.75	49,49,50,50	0
3	CO3	A	600	4/4	0.28	-1.07	43,44,44,44	0
3	CO3	H	600	4/4	0.14	-1.16	49,49,50,50	0
3	CO3	I	600	4/4	0.13	-1.37	49,49,50,50	0
3	CO3	G	600	4/4	0.14	-1.57	49,50,50,50	0
3	CO3	C	600	4/4	0.18	-2.04	43,44,44,44	0
2	FE	F	500	1/1	0.09	-2.27	43,43,43,43	0
2	FE	G	500	1/1	0.07	-2.86	44,44,44,44	0
2	FE	A	500	1/1	0.13	-2.97	39,39,39,39	0
2	FE	H	500	1/1	0.06	-3.03	44,44,44,44	0
2	FE	E	500	1/1	0.09	-3.06	43,43,43,43	0
2	FE	D	500	1/1	0.07	-4.16	44,44,44,44	0
3	CO3	B	600	4/4	0.18	-4.80	43,44,44,44	0
2	FE	I	500	1/1	0.07	-4.96	43,43,43,43	0
2	FE	B	500	1/1	0.14	-5.52	39,39,39,39	0
2	FE	C	500	1/1	0.09	-5.95	39,39,39,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.